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(54) **CRYSTAL STRUCTURE OF HUMAN JAK3 KINASE DOMAIN COMPLEX AND BINDING POCKETS THEREOF**

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(51) **Int. Cl.**

C12Q 1/00	(2006.01)
G01N 33/53	(2006.01)
C12Q 1/48	(2006.01)
C12N 9/00	(2006.01)
C12N 9/12	(2006.01)
G01N 31/00	(2006.01)
G06G 7/58	(2006.01)

(52) **U.S. Cl.**

USPC **703/11**; 435/7.6; 435/7.71; 435/15; 435/183; 435/194; 435/4; 702/27

(58) **Field of Classification Search**

None

See application file for complete search history.

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(57) **ABSTRACT**

The present invention relates to human Janus Kinase 3 (JAK3) and JAK3-like binding pockets. The present invention provides a computer comprising a data storage medium encoded with the structure coordinates of such binding pockets. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for and design compounds, including inhibitory compounds, that bind to JAK3 protein or JAK3 protein homologues, or complexes thereof. The invention also relates to crystallizable compositions and crystals comprising JAK3 kinase domain and JAK3 kinase domain complexes with AMP-PNP.

4 Claims, 9 Drawing Sheets

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Figure 1

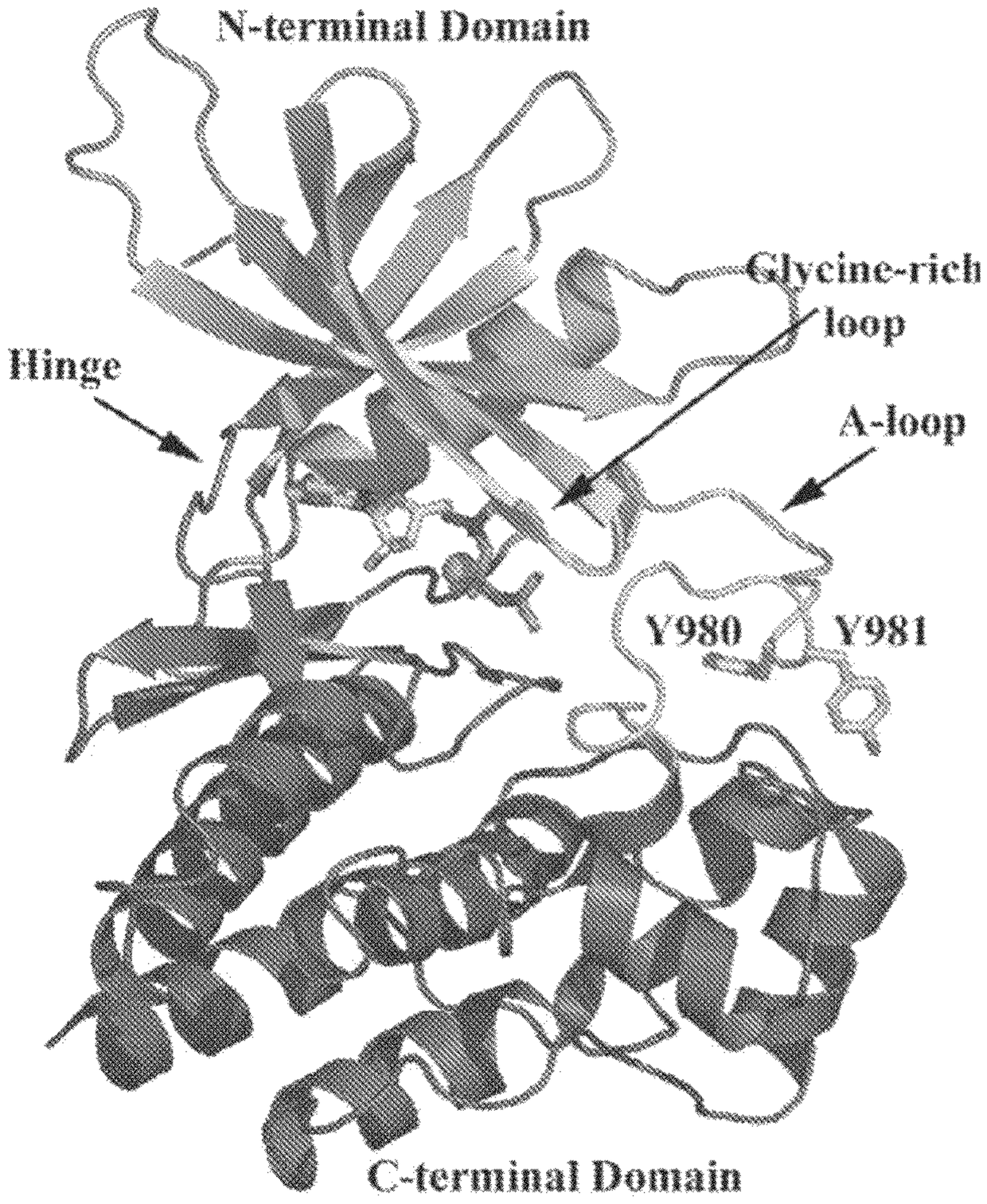

N-terminal Domain
Glycine-rich loop
Hinge
A-loop
Y980
Y981
C-terminal Domain

Figure 2

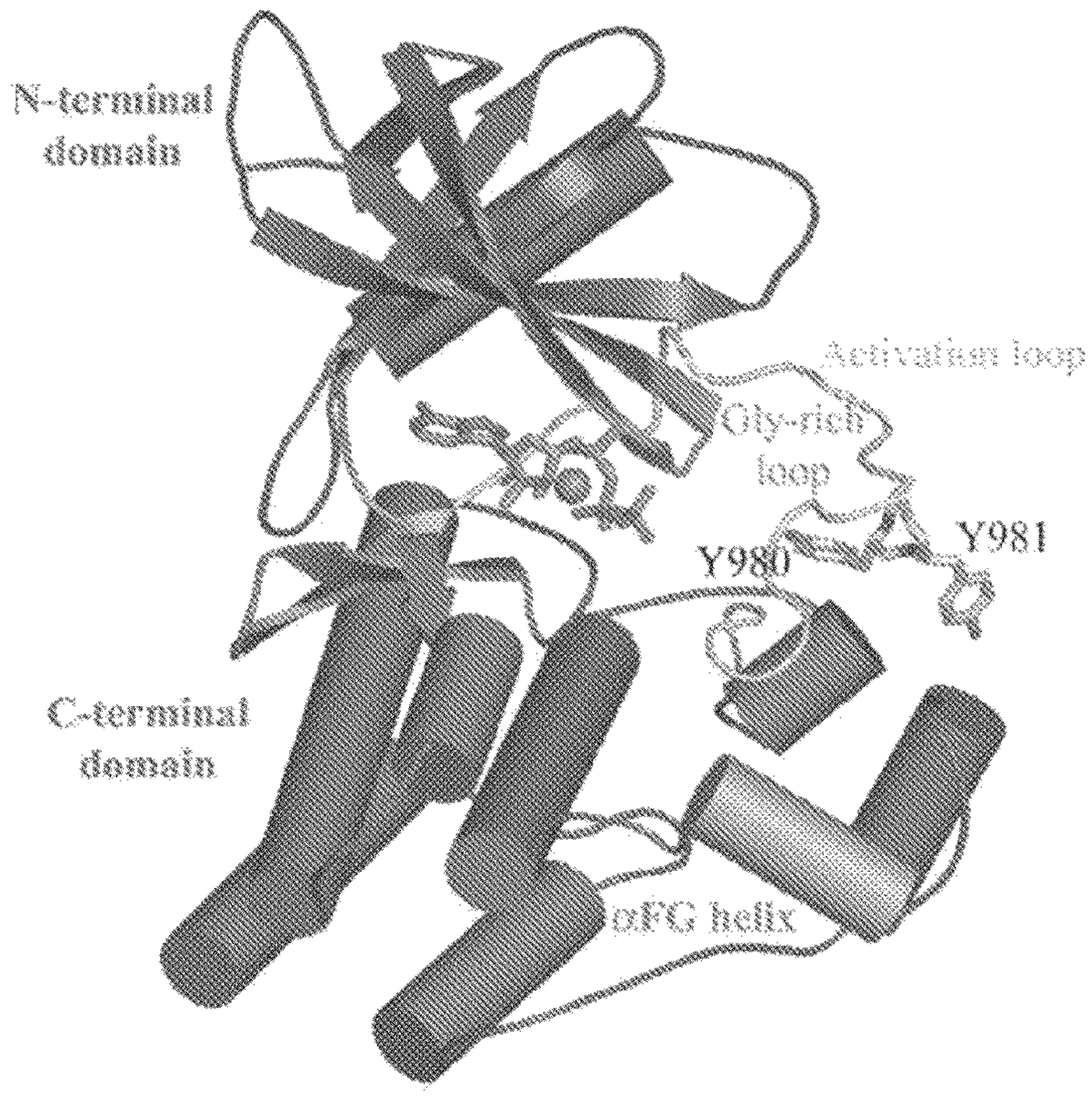

N-terminal domain
Activation loop
Gly-rich loop
Y981
Y980
C-terminal domain
αFG helix

Figure 3

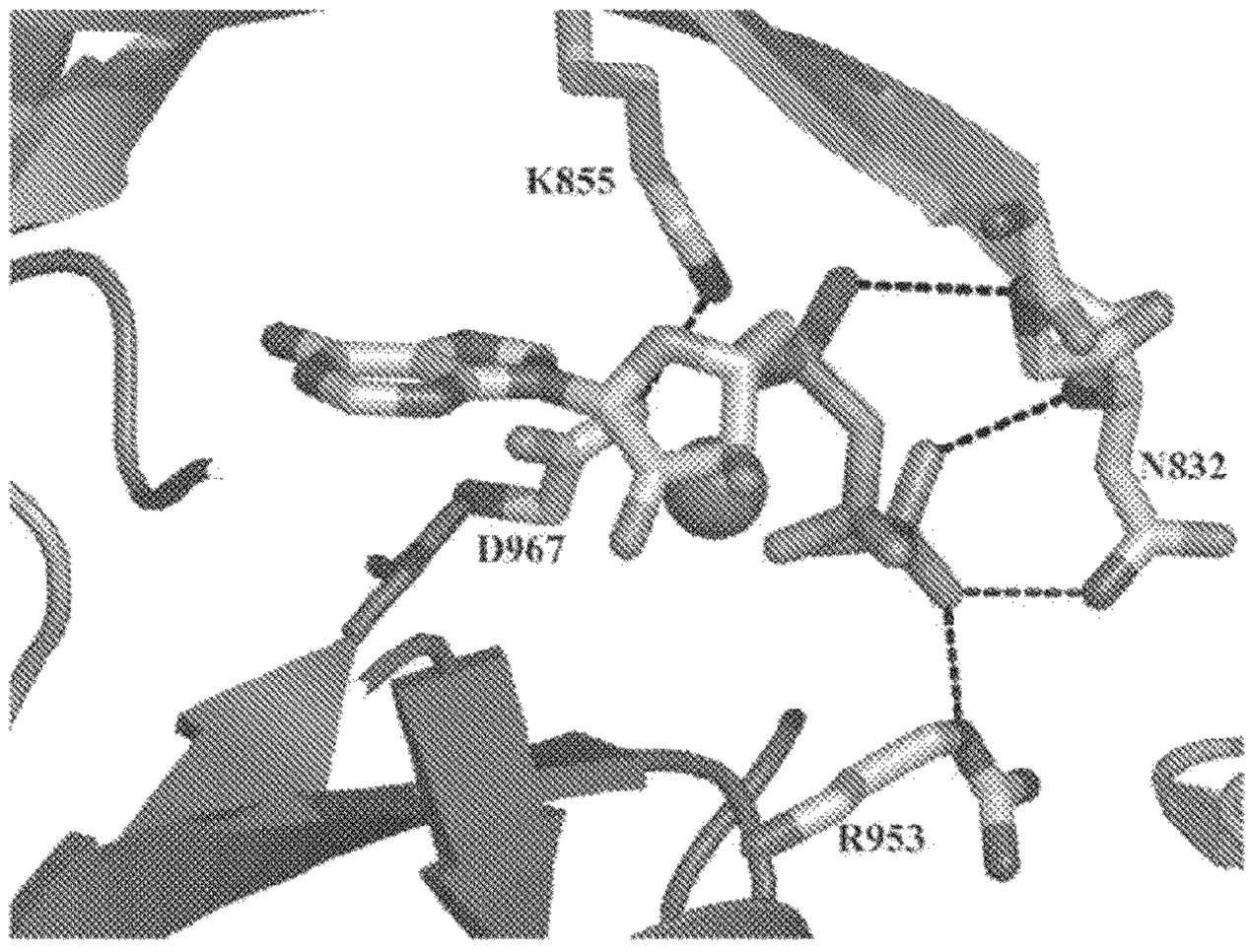


Figure 4

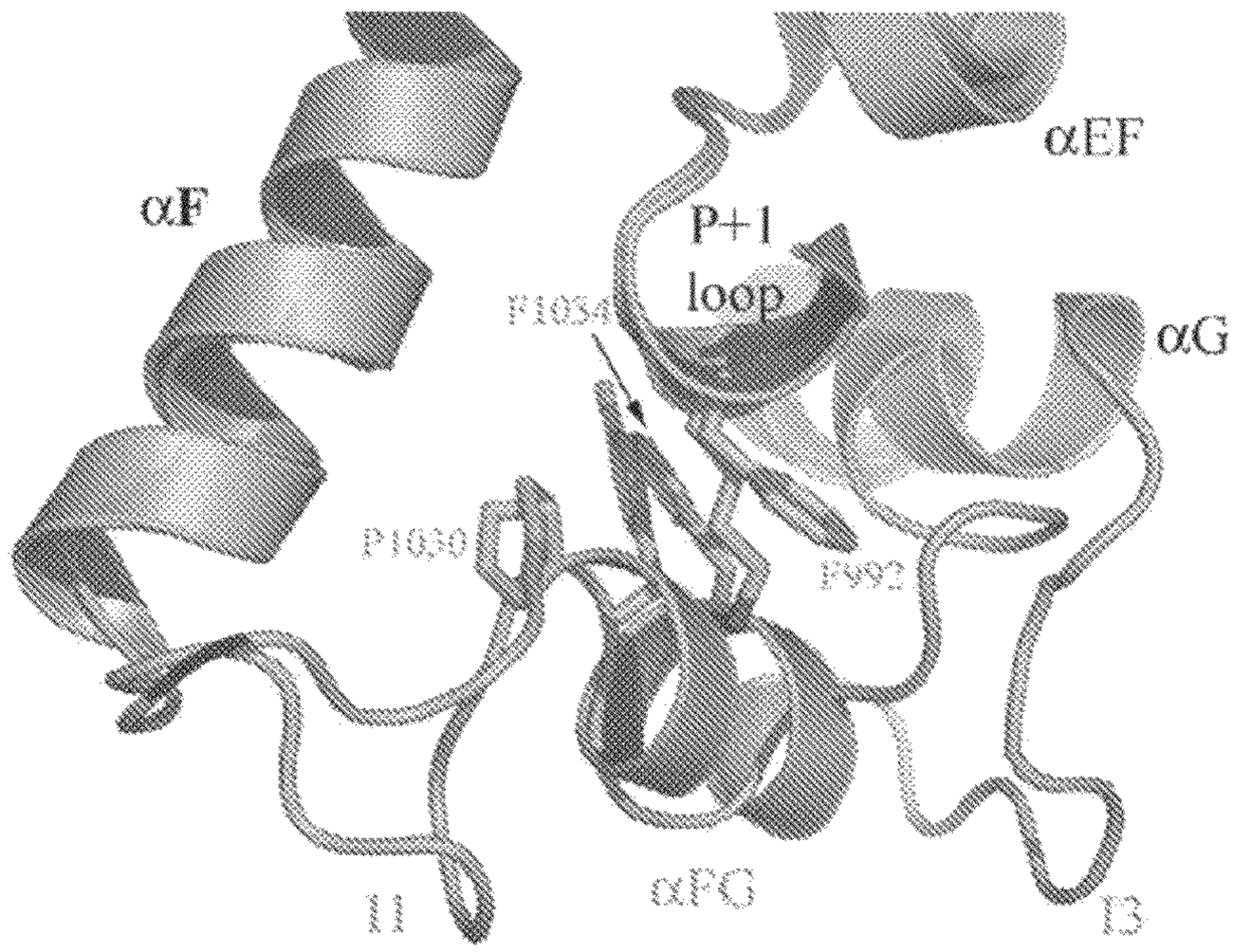
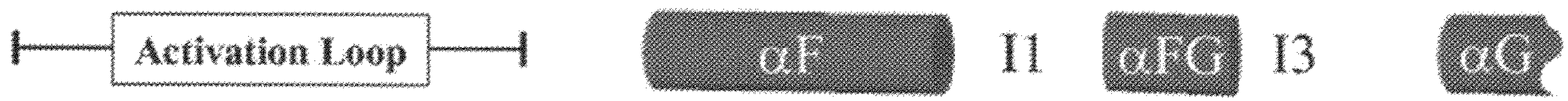


Figure 5

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Jak3    967  DFGLAKLLPLDKDYYVVREPGQSPIFWYAPESLSDNIFSRQSDVWSFGVVLYELFTYCDKSC-SPSAEFLRMMGCERDVPA----LCRLLE
Ack     270  DFGLMRALPQNDDHYVMQEHRKVPFAWCAPESLKTRTFSHASDTWMFGVTLWEMFTYG----QEP---W----------------IGLNGSQILH
MuSK    742  DFGLSRNI-YSADYYKDA----IPIRWMPPESIFYNRYTTESDVWAYGVVLWEIFSYG----LQP---Y----------------YGMAHEEVIY
Insr   1150  DFGMTRDI-YETDYYRKGGKGLLPVRWMAPESLKDGVFTTSSDMWSFGVVLWEITSLA----EQP---Y----------------QGLSNEQVLK
FGFR1   641  DFGLARDI-HHIDYYKKTTNGRLPVKWMAPEALFDRIYTHQSDVWSFGVLLWEIFTLG----GSP---Y----------------PGVPVEELFK
c-Src   404  DFGLARLI-EDNEYTARQG-AKFPIKWTAPEAALYGRFTIKSDVWSFGILLTELTTKG----RVP---Y----------------PGMVNREVLD
```

Figure 6

Figure 7

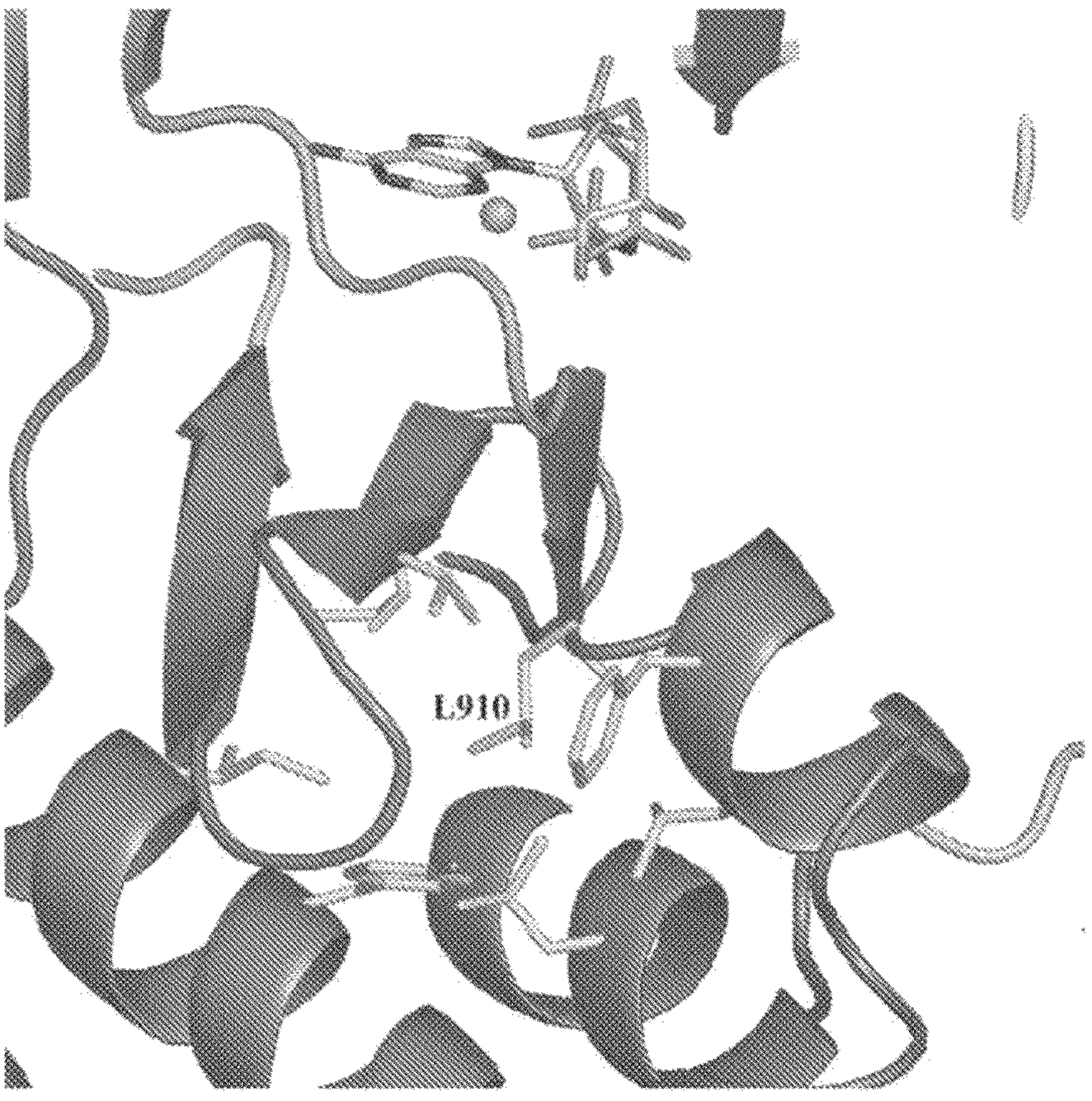


Figure 8

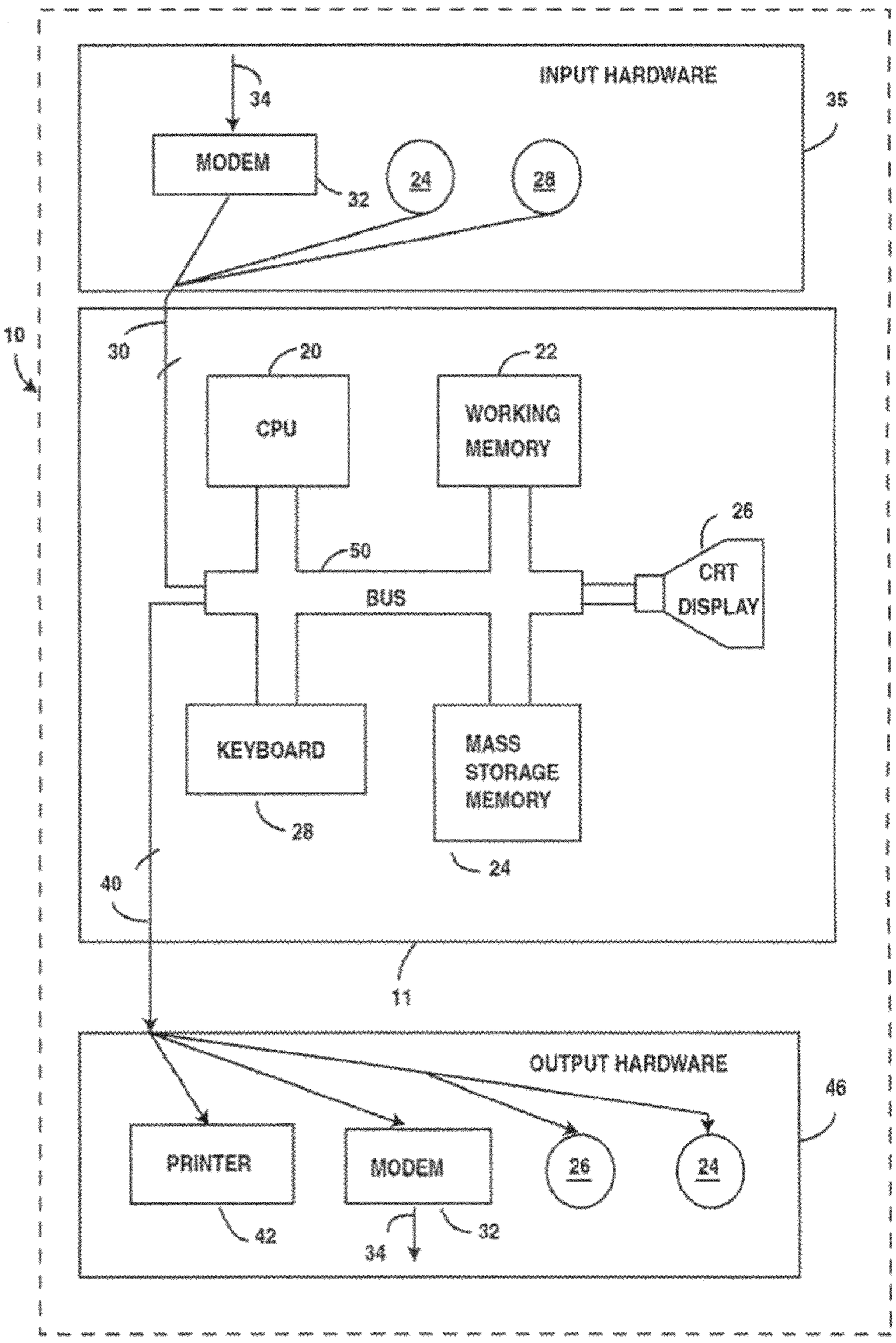

INPUT HARDWARE
35
34
MODEM
32
24
28
10
30
20
22
CPU
WORKING MEMORY
26
50
CRT DISPLAY
BUS
KEYBOARD
MASS STORAGE MEMORY
28
24
40
11
OUTPUT HARDWARE
46
PRINTER
MODEM
26
24
42
34
32

Figure 9

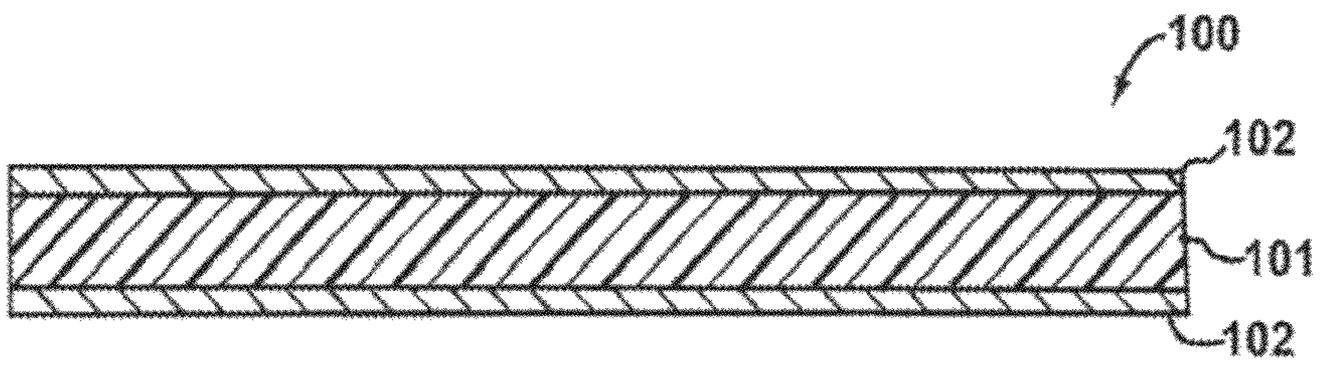
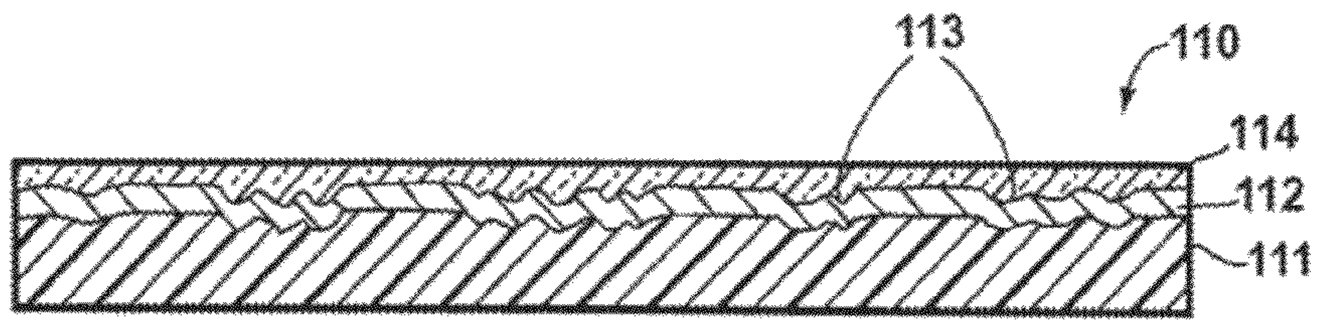


Figure 10



CRYSTAL STRUCTURE OF HUMAN JAK3 KINASE DOMAIN COMPLEX AND BINDING POCKETS THEREOF

This application is a divisional of U.S. application Ser. No. 12/471,896, filed May 26, 2009, now U.S. Pat. No. 8,192,972; which is a divisional of U.S. application Ser. No. 11/114,979, filed Apr. 26, 2005, now U.S. Pat. No. 7,558,717; which claims priority from Provisional Application No. 60/669,771, filed Apr. 8, 2005 and Provisional Application No. 60/566,393, filed Apr. 28, 2004. Each of these prior applications is incorporated herein by reference.

TECHNICAL FIELD OF INVENTION

The present invention relates to human Janus Kinase 3 (JAK3) and JAK3-like binding pockets. The present invention provides a computer comprising a data storage medium encoded with the structure coordinates of such binding pockets. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for and design compounds, including inhibitory compounds, that bind to JAK3 protein or JAK3 protein homologues, or complexes thereof. The invention also relates to crystallizable compositions and crystals comprising JAK3 kinase domain and JAK3 kinase domain complexes with AMP-PNP.

BACKGROUND OF THE INVENTION

Janus kinases (JAKs) are non-receptor tyrosine kinases that play an essential role in cytokine signaling (Darnell et al., *Science* 264: 1415-1421 (1994); Ihle, *Adv. Immunol.* 60: 1-35 (1995)). The JAK family consists of four evolutionary-conserved mammalian JAK proteins JAK1, JAK2, JAK3 and TYK2, which are each approximately 120 kDa in molecular mass, and homologues in other vertebrates such as chicken, and zebrafish and *drosophila*. These kinases appear to be responsible for the transmission of signal by most cytokines and neurokines (Rane and Reddy, *Oncogene* 19: 5662-5679 (2000)). Accumulated evidence suggests that binding of cytokines to their receptors induces receptor oligomerization, which results in an increased affinity of the cytoplasmic domain of the receptor for the JAK kinases. As a consequence of this increased affinity, the JAK kinases are recruited to the receptors resulting in their phosphorylation and subsequent activation. The activated JAKs then phosphorylate the cytoplasmic tails of the receptors on target tyrosines residues, which in turn serve as the docking sites for the Src-homology-2 (SH2) domains of signal transducer and activation of transcription (STAT) proteins. The recruited STATs are phosphorylated by JAKs on specific tryosine residues, which causes their release from the receptor and finally dimerization through a reciprocal phosphotyrosine-SH2 domain interaction (Chen et al., *Cell* 93:827-839 (1998); Becker et al., *Nature* 394: 145-151 (1998)). The dimerized STAT proteins then translocate to the nucleus where they act as transcription factors.

A unique feature of the domain-structure of JAKs that distinguishes them from other tyrosine kinases, a C-terminal catalytic domain and an immediately preceded pseudokinase domain (Ihle, supra). The pseudokinase domain lacks canonical residues that are essential for catalytic function. Several lines of evidence suggest that this domain regulates catalytic activity and autophosphorylation (Saharinen et al., *Mol. Biol. Cell* 14: 1448-1459 (2003); Saharinen et al., *Mol. Cell. Biol.* 20: 3387-3395 (2000); Saharinen et al., *J. Biol. Chem.* 277: 47954-47963 (2002); Chen et al., *Mol. Cell. Biol.* 20: 947-956 (2000)).

In addition to the two kinase domains, JAKs contain an N-terminal band four-point-one, erzin, radixin, moesin (FERM) homology domain and an SH2-like domain (Girault et al., *Trends Biochem. Sci.* 24: 54-57 (1999)). The FERM domain is a 300-amino acid protein-protein interaction module that mediates receptor interactions and is important for the preservation of proper catalytic function (Terawaki et al., *Acta Crystallog*. D59: 177-179 (2003); Smith et al., *J. Biol. Chem.* 278: 4949-4956 (2003); Hamada et al., *EMBO J.* 19: 4449-4462 (2000); Hamada et al., *EMBO J.* 22: 502-514 (2003); Pearson et al., *Cell* 101: 259-270 (2000); Zhou et al., *Mol. Cell.* 8: 959-969 (2001)).

The activity of JAKs is also regulated by the two tyrosines in the activation loop of the catalytic domain (Gauzzi et al., *J. Biol. Chem.* 271: 20494-20500 (1996); Feng et al., *Mol. Cell. Biol.* 17: 2497-2501 (1997); Zhou et al., *Proc. Natl. Acad. Sci. USA* 94: 13850-13855 (1997)). In JAK3, phosphorylation of Tyr980 and Tyr981 results in positive and negative regulation of its enzymatic activity, respective (Zhou, supra).

JAK3 is predominantly expressed in lymphoid and myeloid cell lines and in hematopoietic tissues such as the thymus, bone marrow, spleen, and fetal liver (Rane and Reddy, *Oncogene* 21:3334-3358 (2002)). In contrast, other JAKs are ubiquitously expressed. JAK3 specifically associates with the common γ chain (γc) of the cytokine receptors for interleukin-2 (IL-2), IL-4, IL-7, IL-9, IL-15 and IL-21 (Kisseleva et al., *Gene* 285:1-24 (2002); O'Shea et al., *Cell* 109 Suppl; S121-131 (2002)). In humans, mutations in JAK3 or γc result in sever combined immunodeficiency (SCID), which is characterized by the absence of circulating mature T cells and natural killer cells, but not B cells (TB^+SCID) (Notarangelo et al., *Hum. Mutat.* 18: 255-263 (2001); Roberts et al., *Blood* 103:2009-2018 (2004); Epub in November 2003). JAK3−/− mice also exhibit severe immunodeficiency (Thomis et al., *Science* 270: 794-797 (1995)).

Therapeutic targeting of JAK3 kinase has received particular attention, because the effects owing to the complete absence of JAK3 are limited to the immune system. Several JAK3 inhibitors, such as JANEX-1, AG-490, WHI-P154 and PNU156804 have been reported (Sudbeck et al., *Clin. Cancer Res.* 5: 1569-1582 (1999); Cetkovic-Cvrlje et al. *Arzeneimittolforschung* 53: 648-654 (2003); Cetkovic-Cvrlje et al., *Clin. Immunol.* 106: 213-225 (2003); Saemann et al., *Transplantation* 75: 1864-1874 (2003); Stepkowski et al., *Blood* 99: 680-689 (2002)). More recently, Pfizer imported an orally active JAK3 selective inhibitor, CP-690,550 as an immunosuppressive agent in mouse and monkey transplant models (Changelian et al., *Science* 302: 875-878 (2003)). Collectively these data suggest that JAK3 is an attractive pharmacologic target for the treatment of immune-mediated transplant rejection Kirken, *Transplant Proc.* 33: 3268-3270 (2001)).

Despite its importance in SCID and as a clinical target for immunosuppression, very little is known about the three-dimensional structure of JAK3. Drug design for human therapy has been hampered because the structure of JAK3 was not previously known. Without structural information of JAK3, the detailed knowledge of the mechanism is limited and progress of designing drugs as specific inhibitors is impeded. Structural information on the unique features of the active site of human JAK3 would facilitate drug discovery.

SUMMARY OF THE INVENTION

The present invention solves the problems identified above by providing for the first time the crystal structure of JAK3-

AMP-PNP complex. This crystal structure of human JAK3 kinase domain in complex with AMP-PNP bound to its ATP-binding site provides important structural information for the development of novel JAK3 selective inhibitors.

The present invention also provides molecules comprising JAK3 binding pockets, or JAK3-like binding pockets that have similar three-dimensional shapes. In one embodiment, the molecules are JAK3 kinase domain complexes. In another embodiment, the molecules are JAK3 kinase domain homologues, or complexes thereof. In another embodiment, the molecules are in crystalline form.

The invention provides crystallizable compositions and crystals comprising JAK3 kinase domain, complexes thereof, or homologues thereof.

The invention provides a computer comprising a machine-readable storage medium, comprising a data storage material encoded with machine-readable data, wherein the data defines the JAK3 or JAK3-like binding pocket or domain according to the structure coordinates of Table 2. Such storage medium when read and utilized by a computer programmed with appropriate software can display, on a computer screen or similar viewing device, a three-dimensional graphical representation of such binding pockets. In one embodiment, the structure coordinates of said binding pocket or domain are produced by homology modeling of at least portion of the coordinates of Table 2.

The invention also provides method for designing, selecting, evaluating and identifying and/or optimizing compounds which bind to the molecules or molecular complexes or their binding pockets. Such compounds are potential inhibitors of JAK3, JAK3-like proteins or its homologues.

The invention also provides a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to JAK3, particular JAK3 homologues. This is achieved by using at least some of the structure coordinates obtained from the JAK3 kinase domain.

The present invention provides a crystal comprising a human Janus Kinase 3 kinase domain.

The present invention provides a crystal comprising a Janus Kinase 3 kinase domain homologue.

The present invention provides a crystal comprising a human Janus Kinase 3 kinase domain complex.

The present invention provides a crystal comprising a Janus Kinase 3 kinase domain homologue complex.

The present invention also provides a crystal comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and a chemical entity selected from the group consisting of adenosine, ATP, an ATP analogue, AMP-PNP, a nucleotide triphosphate, a nucleotide diphosphate, phosphate and active site inhibitor.

The present invention also provides a crystal comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and AMP-PNP.

The present invention also provides a crystal comprising a human Janus Kinase 3 kinase domain; a crystal comprising a human Janus Kinase 3 kinase domain complex; a crystal comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and a chemical entity selected from the group consisting of adenosine, ATP, an ATP analogue, AMP-PNP, a nucleotide triphosphate, a nucleotide diphosphate, phosphate and active site inhibitor; and a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and AMP-PNP; wherein said human Janus Kinase 3 kinase domain is selected from the group consisting of amino acid residues 810-1100 of SEQ ID NO:1, amino acid residues 810-1104 of SEQ ID NO:1, amino acid residues 810-1115 of SEQ ID NO:1, amino acid residues 810-1124 of SEQ ID NO:1, and amino acid residues 813-1100 of SEQ ID NO:1.

The present invention also provides crystal comprising a human Janus Kinase 3 kinase domain; a human Janus Kinase 3 kinase domain complex; a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and a chemical entity selected from the group consisting of adenosine, ATP, an ATP analogue, AMP-PNP, a nucleotide triphosphate, a nucleotide diphosphate, phosphate and active site inhibitor; and a crystal comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and AMP-PNP; wherein said human Janus Kinase 3 kinase domain is amino acid residues 810-1115 of SEQ ID NO:1.

The present invention provides a crystallizable composition comprising a human Janus Kinase 3 kinase domain.

The present invention provides a crystallizable composition comprising a Janus Kinase 3 kinase domain homologue.

The present invention provides a crystallizable composition comprising a human Janus Kinase 3 kinase domain complex.

The present invention provides a crystallizable composition comprising a Janus Kinase 3 kinase domain homologue complex.

The present invention provides a crystallizable composition comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and a chemical entity selected from the group consisting of adenosine, ATP, an ATP analogue, AMP-PNP, a nucleotide triphosphate, a nucleotide diphosphate, phosphate and active site inhibitor.

The present invention also provides a crystallizable composition comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and AMP-PNP.

The present invention also provides a crystallizable composition comprising a human Janus Kinase 3 kinase domain; a crystallizable composition comprising a human Janus Kinase 3 kinase domain complex; a crystallizable composition comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and a chemical entity selected from the group consisting of adenosine, ATP, an ATP analogue, AMP-PNP, a nucleotide triphosphate, a nucleotide diphosphate, phosphate and active site inhibitor; and a crystallizable composition comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and AMP-PNP, wherein said human Janus Kinase 3 kinase domain is selected from the group consisting of amino acid residues 810-1100 of SEQ ID NO:1, amino acid residues 813-1104 of SEQ ID NO:1, amino acid residues 810-1115 of SEQ ID NO:1, amino acid residues 810-1124 of SEQ ID NO:1, and amino acid residues 813-1100 of SEQ ID NO:1.

The present invention also provides a crystallizable composition comprising a human Janus Kinase 3 kinase domain; a crystallizable composition comprising a human Janus

Kinase 3 kinase domain complex; a crystallizable composition comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and a chemical entity selected from the group consisting of adenosine, ATP, an ATP analogue, AMP-PNP, a nucleotide triphosphate, a nucleotide diphosphate, phosphate and active site inhibitor; and a crystallizable composition comprising a human Janus Kinase 3 kinase domain complex, wherein said human Janus Kinase 3 kinase domain complex comprises human Janus Kinase 3 kinase domain and AMP-PNP, wherein said human Janus Kinase 3 kinase domain is amino acid residues 810-1115 of SEQ ID NO:1.

The present invention provides a computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data and a means for generating three-dimensional structural information of said binding pocket or domain; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket or domain, or information produced using said three-dimensional structural information of said binding pocket or domain.

The present invention also provides a computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data and a means for generating three-dimensional structural information of said binding pocket or domain; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket or domain, or information produced using said three-dimensional structural information of said binding pocket or domain,

wherein the binding pocket is produced by homology modeling of the structure coordinates of said Janus Kinase 3 amino acid residues according to Table 2.

The present invention also provides a computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data and a means for generating three-dimensional structural information of said binding pocket or domain; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket or domain, or information produced using said three-dimensional structural information of said binding pocket or domain,

wherein said means for generating three-dimensional structural information is provided by means for generating a three-dimensional graphical representation of said binding pocket or domain.

The present invention also provides a computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data and a means for generating three-dimensional structural information of said binding pocket or domain; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket or domain, or information produced using said three-dimensional structural information of said binding pocket or domain,

wherein said output hardware is a display terminal, a printer, CD or DVD recorder, ZIP™ or JAZ™ drive, a disk drive, or other machine-readable data storage device.

The present invention provides a method of using a computer for selecting an orientation of a chemical entity that interacts favorably with a binding pocket or domain selected from the group consisting of;

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket or domain thereof on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket or domain;

(c) quantifying the association between said chemical entity and all or part of the binding pocket or domain for different orientation of the chemical entity; and

(d) selecting the orientation of the chemical entity with the most favorable interaction based on said quantified association.

The present invention also provides a method of using a computer for selecting an orientation of a chemical entity that interacts favorably with a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket or domain thereof on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket or domain;

(c) quantifying the association between said chemical entity and all or part of the binding pocket or domain for different orientations of the chemical entity; and

(d) selecting the orientation of the chemical entity with the most favorable interaction based on said quantified association,

further comprising generating a three-dimensional graphical representation of the binding pocket or domain prior to step (b).

The present invention also provides a method of using a computer for selecting an orientation of a chemical entity that interacts favorably with a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884,

Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket or domain thereof on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket or domain;

(c) quantifying the association between said chemical entity and all or part of the binding pocket or domain for different orientations of the chemical entity; and

(d) selecting the orientation of the chemical entity with the most favorable interaction based on said quantified association,

wherein energy minimization, molecular dynamics simulations, or rigid-body minimizations are performed simultaneously with or following step (b).

The present invention also provides a method of using a computer for selecting an orientation of a chemical entity that interacts favorably with a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket or domain thereof on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket or domain;

(c) quantifying the association between said chemical entity and all or part of the binding pocket or domain for different orientations of the chemical entity; and

(d) selecting the orientation of the chemical entity with the most favorable interaction based on said quantified association,

further comprising the steps of:

(e) repeating steps (b) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that interacts more favorably with said binding pocket or domain based on said quantified association of said first or second chemical entity.

The present invention provides a method of using a computer for selecting an orientation of a chemical entity with a favorable shape complementarity in a binding pocket consisting of a set of amino acid residues that are identical to human Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket and all or part of the ligand bound therein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket;

(c) quantitating the contact score of said chemical entity in different orientations; and

(d) selecting an orientation with the highest contact score.

The present invention also provides a method of using a computer for selecting an orientation of a chemical entity with a favorable shape complementarity in a binding pocket consisting of a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket and all or part of the ligand bound therein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket;

(c) quantitating the contact score of said chemical entity in different orientations; and

(d) selecting an orientation with the highest contact score,

further comprising generating a three-dimensional graphical representation of the binding pocket and all or part of the ligand bound therein prior to step (b).

The present invention also provides a method of using a computer for selecting an orientation of a chemical entity with a favorable shape complementarity in a binding pocket consisting of a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket and all or part of the ligand bound therein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket;

(c) quantitating the contact score of said chemical entity in different orientations; and

(d) selecting an orientation with the highest contact score, further comprising the steps of:

(e) repeating steps (b) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that has a higher contact score based on said quantitated contact score of said first or second chemical entity.

The present invention provides a method for identifying a candidate inhibitor of a molecule or molecular complex comprising a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

comprising the steps of:

(a) using a three-dimensional structure of the binding pocket or domain to design, select or optimize a plurality of chemical entities;

(b) contacting each chemical entity with the molecule or the molecular complex;

(c) monitoring the inhibition to the catalytic activity of the molecule or molecular complex by each chemical entity; and

(d) selecting a chemical entity based on the inhibitory effect of the chemical entity on the catalytic activity of the molecule or molecular complex.

The present invention provides a method of designing a compound or complex that interacts with a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues that are identical to human Janus kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.5 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues according to Table 2, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not more than about 3.0 Å;

comprising the steps of:

(a) providing the structure coordinates of said binding pocket or domain on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) using the computer to dock a first chemical entity in part of the binding pocket or domain;

(c) docking at least a second chemical entity in another part of the binding pocket or domain;

(d) quantifying the association between the first or second chemical entity and part of the binding pocket or domain;

(e) repeating steps (b) to (d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity;

(f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to the binding pocket or domain on a computer screen using the three-dimensional graphical representation of the binding pocket or domain and said first and second chemical entity; and

(g) assembling the first and second chemical entity into a compound or complex that interacts with said binding pocket or domain by model building.

The present invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex of unknown structure, wherein the molecule is sufficiently homologous to human Janus Kinase 3 kinase domain, comprising the steps of:

(a) crystallizing said molecule or molecular complex;

(b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

(c) applying at least a portion of the structure coordinates set forth in Table 2 or homology model thereof to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown; and

(d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map.

The present invention also provides a method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure, wherein the molecule is sufficiently homologous to human Janus Kinase 3 kinase domain, comprising the steps of:

(a) crystallizing said molecule or molecular complex;

(b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

(c) applying at least a portion of the structure coordinates set forth in Table 2 or homology model thereof to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown; and

(d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map,

wherein the molecule is selected from the group consisting of a Janus Kinase 3 protein and a protein comprising a Janus Kinase 3 kinase domain homologue.

The present invention also provides a method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure, wherein the molecule is sufficiently homologous to human Janus Kinase 3 kinase domain, comprising the steps of:

(a) crystallizing said molecule or molecular complex;

(b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

(c) applying at least a portion of the structure coordinates set forth in Table 2 or homology model thereof to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown; and

(d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map,

wherein the molecular complex is selected from the group consisting of a Janus Kinase 3 protein complex, a Janus Kinase 3 kinase domain complex, and a Janus Kinase 3 kinase domain homologue complex.

The present invention also provides a method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the steps of:

(a) obtaining a crystal comprising said human Janus Kinase 3 kinase protein or said homologue thereof, wherein the crystal is characterized with space group $P2_1$ and has unit cell parameters of a=59.98 Å, b=90.19 Å, c=69.00 Å; β=111.5°;

(b) obtaining the structure coordinates of amino acids of the crystal of step (a), wherein the structure coordinates are set forth in Table 1;

(c) generating a three-dimensional model of said human Janus Kinase 3 kinase protein or said homologue thereof using the structure coordinates of the amino acids obtained in step (b), a root mean square deviation from backbone atoms of said amino acids of not more than ±2.0 Å;

(d) determining a binding site of said human Janus Kinase 3 kinase protein or said homologue thereof from said three-dimensional model; and

(e) performing computer fitting analysis to identify the candidate inhibitor which interacts with said binding site.

The present invention also provides a method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the steps of:

(a) obtaining a crystal comprising said human Janus Kinase 3 kinase protein or said homologue thereof, wherein the crystal is characterized with space group $P2_1$ and has unit cell parameters of a=59.98 Å, b=90.19 Å, c=69.00 Å; β=111.5°;

(b) obtaining the structure coordinates of amino acids of the crystal of step (a), wherein the structure coordinates are set forth in Table 1;

(c) generating a three-dimensional model of said human Janus Kinase 3 kinase protein or said homologue thereof using the structure coordinates of the amino acids obtained in step (b), a root mean square deviation from backbone atoms of said amino acids of not more than ±2.0 Å;

(d) determining a binding site of said human Janus Kinase 3 kinase protein or said homologue thereof from said three-dimensional model; and

(e) performing computer fitting analysis to identify the candidate inhibitor which interacts with said binding site,

further comprising the step of:

(f) contacting the identified candidate inhibitor with said human Janus Kinase 3 kinase protein or said homologue thereof in order to determine the effect of the inhibitor on human Janus Kinase 3 kinase protein activity.

The present invention also provides a method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the steps of:

(a) obtaining a crystal comprising said human Janus Kinase 3 kinase protein or said homologue thereof, wherein the crystal is characterized with space group $P2_1$ and has unit cell parameters of a=59.98 Å, b=90.19 Å, c=69.00 Å; β=111.5°;

(b) obtaining the structure coordinates of amino acids of the crystal of step (a), wherein the structure coordinates are set forth in Table 1;

(c) generating a three-dimensional model of said human Janus Kinase 3 kinase protein or said homologue thereof using the structure coordinates of the amino acids obtained in step (b), a root mean square deviation from backbone atoms of said amino acids of not more than ±2.0 Å,

(d) determining a binding site of said human Janus Kinase 3 kinase protein or said homologue thereof from said three-dimensional model; and

(e) performing computer fitting analysis to identify the candidate inhibitor which interacts with said binding site,

wherein the binding site said human Janus Kinase 3 kinase protein or said homologue thereof determined in step (d) comprises the structure coordinates according to Table 1 of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952,

Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Glu985, Glu988, Scr989, Pro990 and Trp 993, wherein the root mean square deviation from the backbone atoms of said amino acids is not more than ±2.0 Å.

The present invention also provides a method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the steps of:

(a) obtaining a crystal comprising said human Janus Kinase 3 kinase protein or said homologue thereof, wherein the crystal is characterized with space group $P2_1$ and has unit cell parameters of a=59.98 Å, b=90.19 Å, c=69.00 Å; β=111.5°;

(b) obtaining the structure coordinates of amino acids of the crystal of step (a);

(c) generating a three-dimensional model of said human Janus Kinase 3 kinase protein or said homologue thereof using the structure coordinates of the amino acids obtained in step (b), a root mean square deviation from backbone atoms of said amino acids of not more than ±2.0 Å;

(d) determining a binding site of said human Janus Kinase 3 kinase protein or said homologue thereof from said three-dimensional model; and

(e) performing computer fitting analysis to identify the candidate inhibitor which interacts with said binding site.

The present invention also provides a method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the steps of:

(a) obtaining a crystal comprising said human Janus Kinase 3 kinase protein or said homologue thereof, wherein the crystal is characterized with space group $P2_1$ and has unit cell parameters of a=59.98 Å, b=90.19 Å, c=69.00 Å; β=111.5°;

(b) obtaining the structure coordinates of amino acids of the crystal of step (a);

(c) generating a three-dimensional model of said human Janus Kinase 3 kinase protein or said homologue thereof using the structure coordinates of the amino acids generated in step (b), a root mean square deviation from backbone atoms of said amino acids of not more than ±2.0 Å;

(d) determining a binding site of said human Janus Kinase 3 kinase protein or said homologue thereof from said three-dimensional model; and

(e) performing computer fitting analysis to identify the candidate inhibitor which interacts with said binding site,

further comprising the step of:

(f) contacting the identified candidate inhibitor with said human Janus Kinase 3 kinase protein or said homologue thereof in order to determine the effect of the inhibitor on human Janus Kinase 3 kinase protein activity.

The present invention also provides a method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the steps of:

(a) obtaining a crystal comprising said human Janus Kinase 3 kinase protein or said homologue thereof, wherein the crystal is characterized with space group $P2_1$ and has unit cell parameters of a=59.98 Å, b=90.19 Å, c=69.00 Å; β=111.5%

(b) obtaining the structure coordinates of amino acids of the crystal of step (a);

(c) generating a three-dimensional model of said human Janus Kinase 3 kinase protein or said homologue thereof using the structure coordinates of the amino acids generated in step (b), a root mean square deviation from backbone atoms of said amino acids of not more than ±2.0 Å;

(d) determining a binding site of said human Janus Kinase 3 kinase protein or said homologue thereof from said three-dimensional model; and

(e) performing computer fitting analysis to identify the candidate inhibitor which interacts with said binding site,

wherein the binding site of said human Janus Kinase 3 kinase protein or said homologue thereof determined in step (d) comprises the structure coordinates according to Table 1 of a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Glu985, Glu988, Ser989, Pro990 and Trp993, wherein the root mean square deviation from the backbone atoms of said amino acids is not more than ±2.0 Å.

The present invention also provides the method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the step of determining a binding site of said human Janus Kinase 3 kinase protein or the homologue thereof from a three-dimensional model to design or identify the candidate inhibitor which interacts with said binding site.

The present invention also provides a method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the step of determining a binding site of said human Janus Kinase 3 kinase protein or the homologue thereof from a three-dimensional model to design or identify the candidate inhibitor which interacts with said binding site,

wherein the binding site of said human Janus Kinase 3 kinase protein or said homologue thereof determined comprises the structure coordinates according to Table 1 of a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Glu985, Glu988, Ser989, Pro990 and Trp 993, wherein the root mean square deviation from the backbone atoms of said amino acids is not more than ±2.0 Å.

The present invention also provides a method for identifying a candidate inhibitor of a molecule or molecular complex comprising a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues which are identical to human Janus Kinase 3 kinase a set of amino acid resides that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949,

Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 1, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues and said human Janus Kinase 3 amino acid residues is not greater than about 2.0 Å; and

(ii) a set of amino acid residues that are identical to human Janus Kinase 3 kinase amino acid residues according to Table 1, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 kinase amino acid residues is not more than about 3.0 Å; comprising the steps of:

(a) using a three-dimensional structure of the binding pocket or domain to design, select or optimize a plurality of chemical entities; and

(b) selecting said candidate inhibitor based on the inhibitory effect of said chemical entities a human Janus Kinase 3 kinase protein or a human Janus Kinase 3 kinase protein homologue on the catalytic activity of the molecule or molecular complex.

The present invention also provides a method of using a crystal comprising a human Janus Kinase 3 kinase domain and a crystal comprising a Janus Kinase 3 kinase domain homologue in an inhibitor screening assay comprising:

(a) selecting a potential inhibitor by performing rational drug design with a three-dimensional structure determined for the crystal, wherein said selecting is performed in conjunction with computer modeling;

(b) contacting the potential inhibitor with a kinase; and

(c) detecting the ability of the potential inhibitor for inhibiting the kinase.

BRIEF DESCRIPTION OF THE FIGURES

FIG. **1** depicts a ribbon diagram of the overall fold of the JAK3-AMP-PNP complex. The N-terminal and the C-terminal domains are colored light gray and dark gray, respectively. The N-terminal domain, the C-terminal domain, the glycine-rich loop or P-loop which contains the G-X-G-X-X-G motif (SEQ ID NO: 7) in the N-terminal lobe, the hinge region between the N- and C-terminal domains, and the activation loop or A-loop in the C-terminal domain are labeled. The AMP-PNP is shown in a stick representation, and the magnesium ion is represented by a sphere. The two tyrosines which have been shown to be phosphorylated (Y980 and Y981) are on the A-loop and are shown in sticks representation and labeled.

FIG. **2** depicts the overall structure of the Jak3-AMP-PNP complex. The structure is shown with β-sheets as arrows and the α-helices are cylinders. The N-terminal lobe is shown with the glycine rich loop. The C-terminal lobe is shown with the activation loop. The α-FG helix is labeled. The non-hydrolyzable ATP analogue, AMP-PNP, is shown as ball-and-stick format, in the active site. The sites of phosphorylation located in the activation loop, Tyr980 and Tyr981, are shown. All structural figures were prepared with Pymol (DeLano W. L. (2002), DeLano Scientific, San Carlos, Calif., USA).

FIG. **3** shows a detailed representation of the active site of JAK3 with AMP-PNP depicting some of the hydrogen bonds formed between the AMP-PNP and amino acid sidechains of JAK3 as dashed-lines. The bond between the catalytic amino acid residue K855 and D967 is also shown as a dashed-line.

FIG. **4** shows αF and αG of Jak3 were superimposed on c-Src. The I1 and I3 regions jut out from this area. This is perhaps an area for either intra or inter protein-protein interactions. The proximity of the α-FG region to the activation loop suggests that it may play a role in the activation of Jak3.

FIG. **5** shows the α-FG region is unique to Janus kinases. The sequence between αF and αG is conserved in the janus kinases and unique among the other tyrosine kinases. The aligned sequences of Jak3 (amino acid residues 967-1052 of SEQ ID NO: 1) with a variety of other tyrosine kinases, including Ack (SEQ ID NO: 2); MuSK (SEQ ID NO: 3); Insr (SEQ ID NO: 4); FGFR1 (SEQ ID NO: 5); c-Src (SEQ ID NO: 6). The sequences were aligned using the "Align and Superpose" option in Quanta, and then manually aligned based on the resultant structural superposition. The bold black residue corresponds to the residue in the P+1 loop that is typical an arginine or lysine in all tyrosine kinases except the four mammalian Jaks and the closely related 2 Ack kinases, Ack1 and Tnk1.

FIG. **6** shows interactions between inactivated Jak3 and AMP-PNP in the ATP-binding site. Interactions between Jak3 and AMP-PNP in the ATP-binding site. The protein backbone is depicted as a thin coil. Fo-Fc experimental electron density for the inhibitor is shown in a wire lines, contoured at 2.0σ at 2.5 Å resolution.

FIG. **7** shows the location of SCID mutation L910S. Leucine 910 is located at the beginning of the αD helix and is surrounded by a number of other hydrophobic residues from adjoining parts of the C-lobe. Burying a polar sidechain, serine 910, in this hydrophobic pocket would probably lead to disruption of this region of the protein. The results could be the disruption of ATP, substrate binding, or both, resulting in a nonfunctioning kinase. The sidechains of L910 and the surrounding residues are shown.

FIG. **8** shows a diagram of a system used to carry out the instructions encoded by the storage medium of FIGS. **9** and **10**.

FIG. **9** shows a cross section of a magnetic storage medium.

FIG. **10** shows a cross section of a optically-readable data storage medium.

DESCRIPTION OF THE INVENTION

In order that the invention described herein may be more fully understood, the following detailed description is set forth.

Throughout the specification, the word "comprise", or variations such as "comprises" or "comprising" will be understood to imply the inclusion of a stated integer or groups of integers but not exclusion of any other integer or groups of integers.

The following abbreviations are used throughout the application:

A =	Ala =	Alanine	T =	Thr =	Threonine
V =	Val =	Valine	C =	Cys =	Cysteine
L =	Leu =	Leucine	Y =	Tyr =	Tyrosine
I =	Ile =	Isoleucine	N =	Asn =	Asparagine
P =	Pro =	Proline	Q =	Gln =	Glutamine
F =	Phe =	Phenylalanine	D =	Asp =	Aspartic Acid
W =	Trp =	Tryptophan	E =	Glu =	Glutamic Acid
M =	Met =	Methionine	K =	Lys =	Lysine
G =	Gly =	Glycine	R =	Arg =	Arginine
S =	Ser =	Serine	H =	His =	Histidine

Other abbreviations that are used throughout the application include: ANP (for AMP-PNP).

As used herein, the following definitions shall apply unless otherwise indicated.

The term "about" when used in the context of root mean square deviation (RMSD) values takes into consideration the standard error of the RMSD value, which is ±0.1 Å.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a binding pocket or binding site on a protein. The association may be non-covalent—wherein the juxtaposition is energetically favored by hydrogen bonding, hydrophobic, van der Waals or electrostatic interactions—or it may be covalent.

The term "ATP analogue" refers to a compound derived from adenosine-5'-triphosphate (ATP). The compound can be adenosine, AMP, ADP, or a non-hydrolyzable analogue, such as, but not limited to AMP-PNP. The analogue may be in complex with magnesium or manganese ions.

The term "binding pocket" refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity. The term "pocket" includes, but is not limited to, a cleft, channel or site. JAK3, JAK3-like molecules or homologues thereof may be binding pockets which include, but are not limited to, peptide or substrate binding sites, and ATP-binding sites. The shape of a binding pocket may be largely pre-formed before binding of a chemical entity, may be formed simultaneously with binding of a chemical entity, or may be formed by the binding of another chemical entity to a different binding pocket of the molecule, which in turn induces a change in shape of the binding pocket.

The term "catalytic active site" or "active site" refers to the portion of the protein kinase to which nucleotide substrates bind. For example, the catalytic active site of JAK3 is at the interface between the N-terminal and C-terminal domains.

The term "chemical entity" refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. The chemical entity can be, for example, a ligand, substrate, nucleotide triphosphate, nucleotide diphosphate, phosphate, nucleotide, agonist, antagonist, inhibitor, antibody, peptide, protein or drug. In one embodiment, the chemical entity is an inhibitor or substrate for the active site.

The term "conservative substitutions" refers to residues that are physically or functionally similar to the corresponding reference residues. That is, a conservative substitution and its reference residue have similar size, shape, electric charge, chemical properties including the ability to form covalent or hydrogen bonds, or the like. Preferred conservative substitutions are those fulfilling the criteria defined for an accepted point mutation in Dayhoff et al., *Atlas of Protein Sequence and Structure,* 5: 345-352 (1978 & Supp.), which is incorporated herein by reference. Examples of conservative substitutions are substitutions including but not limited to the following groups: (a) valine, glycine; (b) glycine, alanine; (c) valine, isoleucine, leucine; (d) aspartic acid, glutamic acid; (e) asparagine, glutamine; (f) serine, threonine; (g) lysine, arginine, methionine; and (h) phenylalanine, tyrosine.

The term "contact score" refers to a measure of shape complementarity between the chemical entity and binding pocket, which is correlated with an RMSD value obtained from a least square superimposition between all or part of the atoms of the chemical entity and all or part of the atoms of the ligand bound (for example, AMP-PNP) in the binding pocket according to Table 2. The docking process may be facilitated by the contact score or RMSD values. For example, if the chemical entity moves to an orientation with high RMSD, the system will resist the motion. A set of orientations of a chemical entity can be ranked by contact score. A lower RMSD value will give a higher contact score. See Meng et al. *J. Comp. Chem.* 4: 505-524 (1992).

The term "corresponds to" to "corresponding amino acid" when used in the context of amino acid residues that correspond to JAK3 amino acid residues refers to particular amino acid residues or analogues thereof in a JAK3 kinase domain homologue that corresponds to amino acid residues in the human JAK3 kinase domain. The corresponding amino acid may be an identical, mutated, chemically modified, conserved, conservatively substituted, functionally equivalent or homologous amino acid residue when compared to the JAK3 amino acid residue to which it corresponds.

Methods for identifying a corresponding amino acid are known in the art and are based upon are sequence, structural alignment, its functional position, or a combination thereof as compared to the JAK3 kinase. For example, corresponding amino acids may be identified by superimposing the backbone atoms of the amino acids in JAK3 and the protein using well known software applications, such as QUANTA (Accelrys, San Diego, Calif. ©2001, 2002). The corresponding amino acids may also be identified using sequence alignment programs such as the "bestfit" program or CLUSTAL W Alignment Tool (Higgins et al., *Methods Enzymol.* 266: 383-402 (1996)).

The term "crystallization solution" refers to a solution that promotes crystallization comprising at least one agent, including a buffer, one or more salts, a precipitating agent, one or more detergents, sugars or organic compounds, lanthanide ions, a poly-ionic compound and/or a stabilizer.

The term "docking" refers to orienting, rotating, translating a chemical entity in the binding pocket, domain, molecule or molecular complex or portion thereof based on distance geometry or energy. Docking may be performed by distance geometry methods that find sets of atoms of a chemical entity that match sets of sphere centers of the binding pocket, domain, molecule or molecular complex or portion thereof. See Meng et al., *J. Comp. Chem.* 4: 505-524 (1992). Sphere centers are generated by providing an extra radius of given length from the atoms (excluding hydrogen atoms) in the binding pocket, domain, molecule or molecular complex or portion thereof. Real-time interaction energy calculations, energy minimizations or rigid-body minimizations (Gschwend et al., *J. Mol. Recognition* 9:175-186 (1996)) can be performed while orienting the chemical entity to facilitate docking. For example, interactive docking experiments can be designed to follow the path of least resistance. If the user in an interactive docking experiment makes a move to increase the energy, the system will resist that move. However, if that user makes a move to decrease energy, the system will favor that move by increased responsiveness. (Cohen et al., *J. Med. Chem.* 33:889-894 (1990)). Docking can also be performed by combining a Monte Carlo search technique with rapid energy evaluation using molecular affinity potentials. See Goodsell and Olsen, *Proteins: Structures, Function and Genetics* 8:195-202 (1990). Software programs that carry out docking functions include but are not limited to MATCHMOL (Cory et al., *J. Mol. Graphics* 2: 39 (1984); MOLFIT (Redington, *Comput. Chem.* 16 216 (1992)) and DOCK (Meng et al., supra).

The term "full-length JAK3" refers to the complete human JAK3 protein (amino acid residues 1 to 1124; SEQ ID NO:1).

The term "generating a three-dimensional structure" or "generating a three-dimensional representation" refers to converting the lists of structure coordinates into structural models or graphical representation in three-dimensional space. This can be achieved through commercially or publicly

available software. A model of a three-dimensional structure of a molecule or molecular complex can thus be constructed on a computer screen by a computer that is given the structure coordinates and that comprises the correct software. The three-dimensional structure may be displayed or used to perform computer modeling or fitting operations. In addition, the structure coordinates themselves, without the displayed model, may be used to perform computer-based modeling and fitting operations.

The term "homologue of JAK3 kinase domain" or "JAK3 kinase domain homologue" refers to a domain that retains JAK3 kinase activity and that has mutations, conservative substitutions, or both, as compared to the human JAK3 kinase domain. In one embodiment, the homologue is at least 95%, 96%, 97%, 98% or 99% identical in sequence to amino acid residues 810-1124 of SEQ ID NO:1, and has conservative substitutions as compared to the JAK3 kinase domain. In another embodiment, the homologue is at least 95%, 96%, 97%, 98% or 99% identical in sequence to amino acid residues 813-1100 of SEQ ID NO:1, and has conservative substitutions as compared to the JAK3 kinase domain. Examples of homologues include but are not limited to the following: the kinase domains of JAK3 from another species or the foregoing, with mutations, conservative substitutions, or both. Such animal species include, but are not limited to, mouse, rat, a primate such as monkey or other primates.

The term "homology model" refers to a structural model derived from know three-dimensional structure(s). Generation of the homology model, termed "homology modeling", can include sequence alignment, residue replacement, residue conformation adjustment through energy minimization, or a combination thereof.

The term "interaction energy" refers to the energy determined for the interaction of a chemical entity and a binding pocket, domain, molecule or molecular complex or portion thereof. Interactions include but are not limited to one or more of covalent interactions, non-covalent interactions such as hydrogen bond, electrostatic, hydrophobic, aromatic, van der Waals interactions, and non-complementary electrostatic, interactions such as repulsive charge-charge, dipole-dipole and charge-dipole interactions. As interactions energies are measured in negative values, the lower the value the more favorable the interaction.

The term "JAK" refers to the kinases from the JAK kinase family. Examples of this family of kinases include but are not limited to JAK3, JAK2, JAK1 and TYK2.

The term "JAK3 ATP-binding pocket" refers to a binding pocket of a molecule or molecular complex defined by the structure coordinates of a certain set of amino acid residues present in the JAK3 structure, as described below. In general, the ligand for the ATP-binding pocket is a nucleotide such as ATP. This binding pocket is in the catalytic active site of the catalytic domain. In the protein kinase family, the ATP-binding pocket is generally located at the interface of the N-terminal and C-terminal domains, and is bordered by the glycine rich loop and the hinge (see, Xie et al., *Structure* 6: 983-991 (1998), incorporated herein by reference).

The term "JAK3 catalytic domain", "JAK3 kinase catalytic domain", "JAK3 protein kinase catalytic domain", "JAK3 catalytic kinase domain" or "JAK3 kinase domain" refers to human JAK3 amino acid residues 810-1115 of SEQ ID NO:1, or the foregoing with additions and deletions of up to 9 amino acid residues at the C-terminal and/or 20 amino acids at the N-terminal of these amino acid residues. The kinase domain includes the catalytic active site.

The term "JAK3 inhibitor-binding pocket" refers to that portion of the JAK3 enzyme active site to which the inhibitor binds. The inhibitor-binding pocket is defined by the structure coordinates of a certain set of amino acid residues present in the JAK3-inhibitor structure.

The term "JAK3-like" refers to all or a portion of a molecule or molecular complex that has a commonality of shape to all or a portion of the JAK3 protein. For example, in the JAK3-like ATP-binding pocket, the commonality of shape is defined by a root mean square deviation of the structure coordinates of the backbone atoms between the amino acids in the JAK3-like ATP-binding pocket and the JAK3 amino acids of the JAK3 ATP-binding pocket, the corresponding amino acid residues in the JAK3-like binding pocket may or may not be identical. Depending on the set of JAK3 amino acid residues that define the JAK3 ATP-binding pocket, one skilled in the art would be able to locate the corresponding amino acid residues, that define a JAK3-like binding pocket in a protein based on sequence or structural homology.

The term "JAK3 protein complex" or "JAK3 homologue complex" refers to a molecular complex formed by associating the JAK3 protein or JAK3 homologue with a chemical entity, for example, a ligand, a substrate, nucleotide triphosphate, nucleotide diphosphate, phosphate, an agonist or antagonist, inhibitor, antibody, drug or compound.

The term "motif" refers to a group of amino acid residues in the JAK3 kinase or homologue that defines a structural compartment or carries out a function in the protein, for example, catalysis, structural stabilization or phosphorylation. The motif may be conserved in sequence, structure and function. The motif can be contiguous in primary sequence or three-dimensional space. Examples of a motif include, but are not limited to, a binding pocket, activation loop, the glycine-rich loop, and the DFG loop (See, Xie et al., *Structure* 6: 983-991 (1998).

The term "part of a binding pocket" refers to less than all of the amino acid residues that define the binding pocket. The structure coordinates of amino acid residues that constitute part of a binding pocket may be specific for defining the chemical environment of the binding pocket, or useful in designing fragments of an inhibitor that may interact with those residues. For example, the portion of amino acid residues may be key residues that play a role in ligand binding, or may be residues that are spatially related and define a three-dimensional compartment of the binding pocket. The amino acid residues may be contiguous or non-contiguous in primary sequence. In one embodiment, part of the binding pocket has at least two amino acid residues, preferably at least three, six, eight, ten, fourteen or fifteen amino acid residues.

The term "part of a JAK3 kinase domain" or "part of a JAK3 kinase domain homologue" refers to less than all of the amino acid residues of a JAK3 kinase domain or kinase domain homologue. In one embodiment part of the JAK3 kinase domain or kinase domain homologue defines the binding pockets, sub-domains, and motifs. The structure coordinates of amino acid residues that constitute part of a JAK3 kinase domain or JAK3 kinase domain homologue may be specific for defining the chemical environment of the protein, or useful in designing fragments of an inhibitor that interact with those residues. The portion of amino acid residues may also be residues that are spatially related and define a three-dimensional compartment of the binding pocket or motif. The amino acid residues may be contiguous or non-contiguous in primary sequence. For example, the portion of amino acid residues may be key residues that play a role in ligand or substrate binding, peptide binding, antibody binding, catalysis, structural stabilization or degradation.

The term "quantified association" refers to calculations of distance geometry and energy. Energy can include but is not limited to interaction energy, free energy and deformation energy. See Cohen, supra.

The term "root mean square deviation" or "RMSD" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of the invention, the "root means square deviation" defines the variation in the backbone atoms of JAK3, a binding pocket, a motif, a domain, or portion thereof, as defined by the structure coordinates of JAK3 described herein. It would be apparent to the skilled worker that the calculation of RMSD involves a standard error of a ±0.1 Å.

The term "soaked" refers to a process in which the crystal is transferred to a solution containing the compound of interest.

The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a protein or protein complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the molecule or molecular complex.

The term "sub-domain" refers to a portion of the domain.

The term "substantially all of a JAK3 binding pocket" or "substantially all of a JAK3 kinase domain" refers to all or almost all of the amino acids in the JAK3 binding pocket or kinase domain. For example, substantially all of a JAK3 binding pocket can be 100%, 95%, 90%, 80%, or 70% of the residues defining the JAK3 binding pocket.

The term "substrate binding pocket" refers to the binding pocket for a substrate of JAK3 or homologue thereof. A substrate is generally defined as the molecule upon which an enzyme performs catalysis. Natural substrates, synthetic substrates or peptides, or mimics of a natural substrate of JAK3 or homologue thereof may associate with the substrate binding pocket.

The term "sufficiently homologous to JAK3" kinase domain refers to a protein that has a sequence identity of at least 25% compared to JAK3 kinase domain. In other embodiments, the sequence identity is at least 40%. In other embodiments, the sequence identity is at least 50%, 60%, 70%, 80%, 90%, 95% 96%, 97%, 98% or 99%.

The term "three-dimensional structural information" refers to information obtained from the structure coordinates. Structural information generated can include the three-dimensional structure or graphical representation of the structure. Structural information can also be generated when subtracting distances between atoms in the structure coordinates, calculating chemical energies for a JAK3 molecule or molecular complex or homologues thereof, calculating or minimizing energies for an association of a JAK3 molecule or molecular complex or homologues thereof to a chemical entity.

Crystallizable Compositions and Crystals of JAK3 Kinase Domain and Complexes Thereof

According to one embodiment, the invention provides a crystal or crystallizable composition comprising a JAK3 kinase domain, a JAK3 kinase domain homologue, a JAK3 kinase domain complex, or a JAK3 kinase domain homologue complex. In one embodiment, the chemical entry is an ATP analogue, nucleotide triphosphate, nucleotide diphosphate, phosphate, adenosine or AMP-PNP. In a certain embodiment, the chemical entity is AMP-PNP.

The JAK3 kinase domain in the crystal or crystallizable composition may be amino acid residues 810-1124 of SEQ ID NO:1, amino acid residues 810-1115 of SEQ ID NO:1, amino acid residues 810-1104 of SEQ ID NO:1, amino acid residues 810-1100 of SEQ ID NO:1 or amino acid residues 813-1100 of SEQ ID NO:1, the JAK3 kinase domain homologue may be the foregoing with conservative substitutions.

SEQ ID NO: 1

```
        10         20         30         40
MAPPSEETPL IPQRSCSLLS TEAGALHVLL PARGPGFFQR

        50         60         70         80
LSFSFGDHLA EDLCVQAAKA SGILPVYHSL FALATEDLSC

        90        100        110        120
WFPPSHIFSV EDASTQVLLY RIRFYFPNWF GLEKCHRFGL

       130        140        150        160
RKDLASAILD LPVLEHLFAQ HRSDLVSGRL PVGLSLKEQG

       170        180        190        200
ECLSLAVLDL ARMAREQAQR PGELLKTVSY KACLPPSLRD

       210        220        230        240
LIQGLSFVTR RRIRRTVRRA LRRVAACQAD RHSLMAKYTM

       250        260        270        280
DLERLDPAGA AETFHVGLPG ALGGHDGLGL LRVAGDGGIA

       290        300        310        320
WTQGEQEVLQ PFCDFPEIVD ISIKQAPRVG PAGEHRLVTV

       330        340        350        360
TRTDNQILEA EFPGLPEALS FVALVDGYFR LTTDSQHFFC

       370        380        390        400
KEVAPPRLLE EVAEQCHGPI TLDFAINKLK TGGSRPGSYV

       410        420        430        440
LRRSPQDFDS FLLTVCVQNP LGPDYKGCLI RRSPTGTFLL

       450        460        470        480
VGLSRPHSSL RELLATCWDG GLHVDGVAVT LTSCCIPRPK

       490        500        510        520
EKSNLIVVQR GHSPPTSSLV QPQSQYQLSQ MTFHKIPADS

       530        540        550        560
LEWHENLGHG SFTKIYRGCR HEVVDGEARK TEVLLKVMDA

       570        580        590        600
KHKNCMESFL EAASLMSQVS YRHLVLLHGV CMAGDSTMVQ

       610        620        630        640
EPVHLGAIDM YLRKRGHLVP ASWKLQVVKQ LAYALNYLED

       650        660        670        680
KGLPHGNVSA RKVLLAREGA DGSPPFIKLS DPGVSPAVLS

       690        700        710        720
LEMLTDRIPW VAPECLREAQ TLSLEADKWG FGATVWEVFS

       730        740        750        760
GVTMPISALD PAKKLQFYED RQQLPAPKWT ELALLIQQCM

       770        780        780        800
AYEPVQRPSF RAVIRDLNSL ISSDYELLSD PTPGALAPRD

       810        820        830        840
GLWNGAQLYA CQDPTIFEER HLKYISQLGK GNFGSVELCR

       850        960        870        880
YDPLGDNTGA LVAVKQLQHS GPDQQRDFQR EIQILKALHS

       890        900        910        920
DFIVKYRGVS YGPGRQSLRL VMEYLPSGCL RDFLQRHRAR

       930        940        950        960
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-continued

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LDASRLLLYS SQICKGMEYL GSRRCVHRDL AARNILVESE

       970        980        990       1000
AHVKIADFGL AKLLPLDKDY YVVREPGQSP IFWYAPESLS

      1010       1020       1030       1040
DINFSRQSDV WSFGVVLYEL FTYCDKSCSP SAEFLRMMGC

      1050       1060       1070       1080
ERDVPALCRL LELLEEGQRL PAPPACPAEV HELMKLCWAP

      1090       1100       1110       1120
SPQDRPSFSA LGPQLDMLWS GSRGCETHAF TAHPEGKHHS LSFS
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In one embodiment, the a crystallizable composition comprises a crystallization solution of equal volumes of JAK3 protein (7.5-30 mg/ml), a salt, a buffer between pH 5.0 and 7.0, 0-10 mM DTT and a polyethylene glycol. The salt includes, but is not limited to KCl, NaCl and $(NH_4)_2SO_4$. The polyethylene glycol includes, but is limited to, PEGMME 550, PEGMME2000, PEG4000, PEG6000. If the crystals are derived from seeding techniques, the concentration of the polyethylene glycol may be less than 20%. In another embodiment, the crystallizable composition comprises a crystallization solution of equal volumes of JAK3 protein (10-15 mg/mL in 50 mM Hepes at pH 8.0, 500 mM NaCl, 20% (v/v) glycerol, 5 mM DTT, and 0.05% (w/v) β-octylglucopyranoside and a solution of 20-26% PEG 3350, 200-260 mM KCl, 20 mM spermine, 10 mM DTT and 100 mM bis-Tris pH 6.0. In one embodiment, the volume of protein used is 0.5 μL. In another embodiment, the volume of protein used in 1.0 μL. In another embodiment, the volume of protein used in 2.0 μL.

Crystals can be grown using sitting drop or hanging drop vapour diffusion techniques, such as, but not limited to techniques described in Example 3. Crystals can be grown in the Corning® 384 Well plate (available from Fisher Scientific), Greiner crystallization low profile plates (available from Hampton Research (Aliso Veijo, Calif.)), both the 96-well CrystalQuick™ standard profile round and flat bottom plates (available from Hampton Research (Aliso Viejo, Calif.)), and the 24 well VDX plates (available from Hampton Research (Aliso Viejo, Calif.)). The volume of the reservoir for the 384-well plate can be 50 μL. The volume of the reservoir for the 96-well low profile plate can be 100 μL, and for the CrystalQuick™ plates it can be varied between 70-100 μL. Crystals can also be grown in 72-well terasaki plates using the microbatch method. They also can be grown in 96-well Corning® (available from Hampton Research (Aliso Viejo, Calif.)) with a reservoir of 50 μL.

According to one embodiment, the invention provides for a crystal with unit cell dimensions of a=59.98 Å b=90.19 Å, c=69.00 Å, α=γ=90, β=111.5° and space group $P2_1$ with 2 molecules in the asymmetric unit. Preferably, the crystal comprises the JAK3-AMP-PNP complex.

According to another embodiment, the invention provides for a crystal with unit cell dimensions of a=72.36 Å b=90.04 Å, c=105.60 Å, α=β=γ=90° and a space $P2_12_12_1$ with 2 molecules in the symmetric unit. Preferably, the crystal comprises the JAK3-AMP-PNP complex.

It will be readily apparent to those skilled in the art that the unit cells of the crystal compositions may deviate up to ±1-4 Å in cell length (and 7-8° in β angle in the $P2_1$ space group) from the above cell dimensions depending on the deviation in the unit calculations or conformational change in the protein.

The JAK3 kinase domain or homologue thereof may be produced by any well-known method, including synthetic methods, such as solid phase, liquid phase and combination solid phase/liquid phase syntheses; recombinant DNA methods, including cDNA cloning, optionally combined with site directed mutagenesis; and/or purification of the natural products. In one embodiment, the protein is overexpressed in baculovirus system.

Methods of Obtaining Crystals of JAK3 Kinase Domain, Complexes Thereof or Homologues Thereof

The invention also relates to a method of obtaining a crystal of JAK3 kinase domain of JAK3 homologue thereof, comprising the steps of:

a) producing and purifying a JAK3 kinase domain or homologue thereof;

b) combining a crystallizable solution with said JAK3 kinase domain or homologue thereof to produce a crystallizable composition; and

c) subjecting said crystallizable composition to conditions which promote crystallization and obtaining said crystals.

The invention also relates to a method of obtaining a crystal of a JAK3 kinase domain complex or JAK3 kinase domain homologue complex, further comprising the step of:

d) soaking said crystal in a buffer solution comprising a chemical entity.

The invention also relates to a method of obtaining a crystal of JAK3 kinase domain complex or JAK3 kinase domain homologue complex, comprising the steps of:

a) producing and purifying a JAK3 kinase domain or homologue thereof;

b) b) combining a crystallizable solution with said JAK3 kinase domain or homologue thereof in the presence of a chemical entity to produce a crystallizable composition; and

c) subjecting said crystallizable composition to conditions which promote crystallization and obtaining said crystals.

In one embodiment, the chemical entity is selected from the group consisting of an ATP analogue, nucleotide triphosphate, nucleotide diphosphate, phosphate, adenosine, AMP-PNP, substrate inhibitor, or active site inhibitor. In another embodiment, the crystallization solution is as described previously. In another embodiment, the composition is treated with micro-crystals of JAK3 kinase domain or JAK3 kinase domain homologues, or complexes thereof.

In certain embodiments, the method of making crystals of JAK3 kinase domain. JAK3 kinase domain homologues, or complexes thereof, includes the use of a device for promoting crystallizations. Devices for promoting crystallization can include but are not limited to the hanging-drop, sitting drop, dialysis or microtube batch devices. (U.S. Pat. Nos. 4,886, 646, 5,096,676, 5,130,105, 5,221,410 and 5,400, 741; Pav et al., *Proteins: Structure, Function, and Genetics* 20: 98-102 (1994), incorporated herein by reference). The hanging-drop, sitting-drop, and some adaptations of the microbatch methods (D'Arcy et al., *J. Cryst. Growth* 168: 175-180 (1996) and Chayen, *J. Appl. Cryst.* 30: 198-202 (1997)) produce crystals by vapor diffusion. The hanging drop and sitting drop containing the crystallizable composition is equilibrated in a reservoir containing a higher or lower concentration of the precipitant. As the drop approaches equilibrium with the reservoir, the saturation of protein in the solution leads to the formation of crystals.

Microseeding or seeding may be used to increase the size and quality of crystals. In this instance, micro-crystals are crushed to yield a stock seed solution. The stock seed solution is diluted in series. Using a needle, glass rod, micro-pipet, micro-loop or strand of hair, a small sample from each diluted solution is added to a set of equilibrated drops containing a

protein concentration equal to or less than a concentration needed to create crystals without the presence of seeds. The aim is to end up with a single seed crystal that will act to nucleate crystal growth in the drop.

In would be readily apparent to one of skill the art to vary the crystallization conditions disclosed above to identify other crystallization conditions that would produce crystals of a JAK3 kinase domain homologue, a JAK3 kinase domain homologue complex, a JAK3 kinase domain or another JAK3 kinase domain complex. Such variations include, but are not limited to, adjusting pH, protein concentration and/or crystallization temperature, changing the identity or concentration of salt and/or precipitant used, using a different method of crystallization, or introducing additives such as detergents (e.g., TWEEN 20 (monolaurate), LDAO, Brij 30 (4 lauryl ether)), sugars (e.g., glucose, maltose), organic compounds (e.g., dioxane, dimethylformamide), lanthanide ions or polyionic compounds that aid in crystallization. High throughput crystallization assays may also be used to assist in finding or optimizing the crystallization condition.

Binding Pockets of JAK3 Kinase Domain or Homologue Thereof

As disclosed herein, applicants have provided the three-dimensional X-ray structure of JAK3-AMP-PNP complex. The atomic coordinates for the structures of JAK3-AMP-PNP complex are presented in Table 2.

To use the structure coordinates generated for the JAK3 complex or one of its binding pockets or homologues thereof, it may be necessary to convert the structure coordinates, or portions thereof, into a three-dimensional shape (i.e., a three-dimensional representation of these complexes or binding pockets). This is achieved through the use of a computer and commercially available software that is capable of generating the three-dimensional representations or structures of molecules or molecular complexes, or portions thereof, from a set of structural coordinates. These three-dimensional representations may be displayed on a computer screen.

Binding pockets, also referred to as binding sites in the present invention, are of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the binding pockets of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or part of the binding pocket. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential inhibitors of the binding pockets of biologically important targets. The binding pockets of this invention will be important for drug design.

The conformations of JAK3 and other proteins at a particular amino acid site, along the polypeptide backbone, can be compared using well-known procedures for performing sequence alignments of the amino acids. Such sequence alignments allow for the equivalent sites on these proteins to be compared. Such methods for performing sequence alignment include, but are not limited to, the "bestfit" program and CLUSTAL W Alignment Tool, Higgins et al., supra.

In one embodiment, the ATP-binding pocket comprises amino acid residues Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Ala853, Lys855, Val884, Met902, Glu903, Tyr904, Leu905, Pro906, Cys909, Arg911, Asp949, Arg953, Asn954, Leu956, Asp967, and Gln988 according to the structure of the JAK3-AMP-PNP complex in Table 2. These amino acid residues are within 5 Å ("5 Å sphere of amino acids") of AMP-PNP bound in the ATP-binding pocket as identified using the program QUANTA (Accelrys, San Diego, Calif. ©2001, 2002).

In another embodiment, the ATP-binding pocket comprises amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to the structure of the JAK3-AMP-PNP complex in Table 2. These amino acid residues are within 8 Å ("8 Å sphere of amino acids") of AMP-PNP bound in the ATP-binding pockets as identified using the program QUANTA (Accelrys, San Diego, Calif. ©2001, 2002).

It will be readily apparent to those of skill in the art that the numbering of amino acid residues in homologues of human JAK3 may be different than that set forth for human JAK3. Corresponding amino acids in JAK3 homologues are easily identified by visual inspection of the amino acid sequences or by using commercially available homology software programs. Homologues of JAK3 include, for example, JAK3 from other species, such as non-humans primates, mouse, rat, etc.

Those of skill in the art understand that set of structure coordinates for an enzyme or an enzyme-complex, or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape. In terms of binding pockets, these variations would not be expected to significantly alter the nature of ligands that could associate with those pockets.

The variations in coordinates discussed above may be generated because of mathematical manipulations of the JAK3-AMP-PNP structure coordinates. For example, the structure coordinates set forth in Table 2 may undergo crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combinations of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal may also account for variations in structure coordinates. If such variations are within a certain root mean square deviation as compared to the original coordinates, the resulting three-dimensional shape is considered encompassed by this invention. Thus, for example, a ligand that bound to the ATP-binding pocket of JAK3 would also be expected to bind to another binding pocket whose structure coordinates defined a shape that fell within the RMSD value.

Various computational analyses may be necessary to determine whether a molecule or binding pocket, or portion thereof, is sufficiently similar to the binding pockets above-described. Such analyses may be carried out in well known software applications, such as ProFit (A.C.R. Martin, ProFit version 1.8, http://www.bioinf.org.uk/software), Swiss-Pdb Viewer (Guex and Peitsch, *Electrophoresis* 18: 2714-2723 (1997)), the Molecular Similarity application of QUANTA (Accelrys, San Diego, Calif. ©2001, 2002) and as described in the accompanying User's Guide, which are incorporated herein by reference.

The above programs permit comparisons between different structures, different conformations of the same structure,

and different parts of the same structure. The procedure used in QUANTA (Accelrys, San Diego, Calif. ©2001, 2002) and Swiss-Pdb Viewer (Guex and Peitsch, *Electrophoresis* 18: 2714-2723 (1997) to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation on the structures; and 4) analyze the results.

The procedure used in ProFit to compare structures includes the following steps: 1) load the structures to be compared; 2) specify selected residues of interest; 3) define the atom equivalences in the selected residues; 4) perform a fitting operation on the selected residues; and 5) analyze the results.

Each structure in the comparison is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QUANTA (Accelrys, San Diego, Calif. ©2001, 2002) is defined by user input, for the purposes of this invention, we will define equivalent atoms as protein backbone atoms N, O, C and Cα for all corresponding amino acid residues between two structures being compared.

The corresponding amino acids may be identified by sequence alignment programs such as the "bestfit" program available from the Genetics Computer Group which uses the local homology algorithm described by Smith and Waterman in *Advances in Applied Mathematics* 2: 482 (1981), which is incorporated herein by reference. A suitable amino acid sequence alignment will require that the proteins being aligned share minimum percentage of identical amino acids. Generally, a first protein being aligned with a second protein should share in excess of about 35% identical amino acids (Hanks et al., *Science* 241: 42 (1988); Hanks and Quinn, *Methods in Enzymology* 200: 38 (1991)). The identification of equivalent residues can also be assisted by secondary structure alignment, for example, aligning the α-helices, β-sheets in the structure. The program Swiss-Pdb viewer (Guex and Peitsch, *Electrophoresis* 18: 2714-2723 (1997) utilizes a best fit algorithm that is based on secondary sequence alignment.

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by the above programs. The Swiss-Pdb Viewer program (Guex and Peitsch, *Electrophoresis* 18: 2714-2723 (1997) sets an RMSD cutoff for eliminating pairs of equivalent atoms that have high RMSD values. An RMSD cutoff value can be used to exclude pairs of equivalent atoms with extreme individual RMSD values. In the program ProFit, the RMSD cutoff value can be specified by the user.

For the purpose of this invention, any molecule, molecular complex, binding pocket, motif, domain thereof or portion thereof that is within a root mean square deviation for backbone atoms (N, Cα, C, O) when superimposed on the relevant backbone atoms described by structure coordinates listed in Table 2 are encompassed by this invention.

One embodiment of this invention provides a crystalline molecule comprising a protein defined by structure coordinates of a set of amino acid residues that are identical to JAK3 amino acid residues according to Table 2, wherein the RMSD between backbone atoms of said set of amino acid residues and said JAK3 amino acid residues is not more than about 3.0 Å. In other embodiments, the RMSD between backbone atoms of said set of amino acid residues and said JAK3 amino acid residues is not greater than about 2.0 Å, not greater than about 1.5 Å, not greater than about 1.1 Å, not greater than about 1.0 Å, not greater than about 0.9 Å, not greater than about 0.8 Å, not greater than about 0.7 Å, not greater than about 0.6 Å, or not greater than about 0.5 Å. Calculations of RMSD values were done with Swiss Pdb Viewer (Guex Peitsch, *Electrophoresis* 18: 2714-2723 (1997)).

In one embodiment, the present invention provides a crystalline molecule comprising all or part of a binding pocket defined by a set of amino acid residues comprising amino acid residues which are identical to human JAK3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993 according to Table 2, wherein the RMSD of the backbone atoms between said JAK3 amino acid residues and said amino acid residues which are identical is not greater than about 2.5 Å. In other embodiments, the RMSD is not greater than about 2.4 Å, 2.2 Å, 2.0 Å, 1.8 Å, 1.6 Å, 1.4 Å, 1.2 Å, 1.0 Å, 0.8 Å, 0.5 Å, 0.3 Å, or 0.2 Å. In other embodiments, the binding pocket is defined by a set of amino acid residues comprising at least four, six, eight, ten, twelve, fifteen, twenty, twenty-five, thirty, thirty-five, forty, forty-five or fifty amino acid residues which are identical to said JAK3 amino acid residues.

Computer Systems

According to another embodiment, this invention provides a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines the above-mentioned molecules or molecular complexes. In one embodiment, the data defines the above-mentioned binding pockets by comprising the structure coordinates of said amino acid residues according to Table 2. To use the structure coordinates generated for JAK3 homologues thereof, or one of its binding pockets, it is at times necessary to convert them into a three-dimensional shape or to extract three-dimensional structural information from them. This is achieved through the use of commercially or publicly available software that is capable of generating a three-dimensional structure or a three-dimensional representation of molecules or portions thereof from a set of structure coordinates. In one embodiment, three-dimensional structure or representation may be displayed graphically.

Therefore, according to another embodiment, this invention provides a machine-readable data storage medium comprising a data storage material encoded with machine readable data. In one embodiment, a machine programmed with instructions for using said data is capable of generating a three-dimensional structure or three-dimensional representation of any of the molecules, or molecular complexes or binding pockets thereof, that are described herein.

This invention also provides a computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines any one of the above molecules or molecular complexes;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit (CPU) coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data and means for generating three-dimensional structural information of said molecule or molecular complex; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said molecule or molecular complex, or information produced by using said three-dimensional structural information of said molecule or molecular complex.

In one embodiment, the data defines the binding pocket of the molecule or molecular complex.

Three-dimensional data generation may be provided by an instruction or set of instructions such as a computer program or commands for generating a three-dimensional structure or graphical representation from structure coordinates, or by subtracting distances between atoms, calculating chemical energies for a JAK3 molecule or molecular complex or homologues thereof, or calculating or minimizing energies for an association of a JAK3 molecule or molecular complex or homologues thereof to a chemical entity. The graphical representation can be generated or displayed by commercially available software programs. Examples of software programs include but are not limited to QUANTA (Accelrys, San Diego, Calif. ©2001, 2002), O (Jones et al., *Acta Crystallogr. A*47: 110-119 (1991)) and RIBBONS (Carson, *J. Appl. Crystallogr.* 24: 958-961 (1991)), which are incorporated herein by reference. Certain software programs may imbue this representation with physico-chemical attributes which are know from the chemical composition of the molecule, such as residue charge, hydrophobicity, torsional and rotational degrees of freedom for the residue or segment, etc. Examples of software programs for calculating chemical energies are described in the Rational Drug Design section.

Information of said binding pocket or information produced by using said binding pocket can be outputted through display terminals, touchscreens, facsimile machines, modems, CD-ROMS, printers, a CD or DVD recorder, ZIP™ or JAZ™ drives or disk drives. The information can be in graphical or alphanumeric form.

In one embodiment, the computer is executing an instruction such as a computer program for generating three-dimensional structure or docking. In another embodiment, the computer further comprises a commercially available software program to display the information as a graphical representation. Examples of software programs include but as not limited to, QUANTA (Accelrys, San Diego, Calif. ©2001, 2002), O (Jones et al., *Acta Crystallogr. A*47: 110-119 (1991)) and RIBBONS (Carson, *J. Appl. Crystallogr.* 24: 958-961 (1991)), all of which are incorporated herein by reference.

FIG. **8** demonstrates one version of these embodiments. System (**10**) includes a computer (**11**) comprising a central processing unit ("CPU") (**20**), a working memory (**22**) which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory (**24**) (such as one or more disk drives, CD-ROM drives or DVD-ROM drives), one or more cathode-ray tube ("CRT") display terminals (**26**), one or more keyboards (**28**), one or more input lines (**30**), and one or more output lines (**40**), all of which are, interconnected by a conventional bi-directional system bus (**50**).

Input hardware (**35**), coupled to computer (**11**) by input lines (**30**), may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems (**32**) connected by a telephone line or dedicated data line (**34**). Alternatively or additionally, the input hardware (**35**) may comprise CD-ROM or DVD-ROM drives or disk drives (**24**). In conjunction with display terminal (**26**), keyboard (**28**) may also be used as an input device.

Output hardware (**46**), coupled to computer (**11**) by output lines (**40**), may similarly be implemented by conventional devices. By way of example, output hardware (**46**) may include CRT display terminal (**26**) for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA (Accelrys, San Diego, Calif. ©2001, 2002) as described herein. Output hardware may also include a printer (**42**), so that hard copy output may be produced, or a disk drive (**24**), to store system output for later use. Output hardware may also include a display terminal, touchscreens, facsimile machines, modems, a CD or DVD recorder, ZIP™ or JAZ™ drives, disk drives, or other machine-readable data storage device.

In operation, CPU (**20**) coordinates the use of the various input and output devices (**35**), (**46**), coordinates data accesses from mass storage (**24**) and accesses to and from working memory (**22**), and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system (**10**) are included as appropriate throughout the following description of the data storage medium.

FIG. **9** shows a cross section of a magnetic data storage medium (**100**) which can be encoded with a machine-readable data that can be carried out by a system such as system (**10**) of FIG. **8**. Medium (**100**) can be a conventional floppy diskette or hard disk, having a suitable substrate (**101**), which may be conventional, and a suitable coating (**102**), which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium (**100**) may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device (**24**).

The magnetic domains of coating (**102**) of medium (**100**) are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system (**10**) of FIG. **8**.

FIG. **10** shows a cross-section of an optically-readably data storage medium (**110**) which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system (**10**) or FIG. **8**. Medium (**110**) can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium (**100**) preferably has a suitable substrate (**111**), which may be conventional, and a suitable coating (**112**), which may be conventional, usually of one side of substrate (**111**).

In the case of CD-ROM, as is well known, coating (**112**) is reflective and is impressed with a plurality of pits (**113**) to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating (**112**). A protective coating (**114**), which preferably is substantially transparent, is provided on top of coating (**112**).

In the case of a magneto-optical disk, as is well known, coating (**112**) has no pits (**113**), but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating (**112**). The arrangement of the domains encodes the data as described above.

In one embodiment, the structure coordinates of said molecules or molecular complexes are provided by homology modeling of at least a portion of the structure coordinates of Table 2. Homology modeling can be used to generate structural models of JAK3 homologues or other homologues pro-

teins based on the known structure of JAK3. This can be achieved by performing one or more of the following steps: performing sequence alignment between the amino acid sequence of a molecule (possibly an unknown molecule) against the amino acid sequence of JAK3; identifying conserved and variable regions by sequence or structure; generating structure coordinates for structurally conserved residues of the unknown structure from those of JAK3; generating conformation for the structurally variable residues in the unknown structure; replacing the non-conserved residues of JAK3 with residues in the unknown structure; building side chain conformations; and refining and/or evaluating the unknown structure.

Software programs that are useful in homology modeling include XALIGN (Wishart et al., *Comput. Appl. Biosci.* 10: 687-688 (1994)) and CLUSTAL W Alignment Tool, Higgins et al., supra. See also, U.S. Pat. No. 5,884,230. These references are incorporated herein by reference.

To perform the sequence alignment, programs such as the "bestfit" program available from the Genetics Computer Group (Waterman in *Advances in Applied Mathematics* 2: 482 (1981), which is incorporated herein by reference) and CLUSTAL W Alignment Tool (Higgins et al., supra, which is incorporated by reference) can be used. To model the amino acid side chains of homologous molecules, the amino acid residues in JAK3 can be replaced, using a computer graphics program such as "O" (Jones et al., *Acta Cryst. Sect. A* 47: 110-119 (1997)), by those of the homologous protein, where they differ. The same orientation or a different orientation of the amino acid can be used. Insertions and deletions of amino acid residues may be necessary where gaps occur in the sequence alignment. However, certain portions of the active site of JAK3 and its homologues are highly conserved with essentially no insertions and deletions.

Homology modeling can be performed using, for example, the computer programs SWISS-MODEL available through Glaxo Wellcome Experimental Research in Geneva, Switzerland; WHATIF available on EMBL servers; Schnare et al., *J. Mol. Biol.* 256: 701-719 (1996); Blundell et al., *Nature* 326: 347-352 (1987); Fetrow and Bryant, *Bio/Technology* 11:479-484 (1993); Greer, *Methods in Enzymology* 202:239-252 (1991); and Johnson et al., *Crit. Rev. Biochem. Mol Biol.* 29: 1-68 (1994). An example of homology modeling can be found, for example, in Szklarz, *Life Sci.* 61: 2507-2520 (1997). These references are incorporated herein by reference.

Thus, in accordance with the present invention, data capable of generating the three-dimensional structure or three-dimensional representation of the above molecules or molecular complexes, or binding pockets thereof, can be stored in a machine-readable storage medium, which is capable of displaying structural information or a graphical three-dimensional representation of the structure. In one embodiment, the means of generating a three-dimensional is provided by the means for generating a three-dimensional structural representation of the binding pocket or protein of a molecule or molecular complex.

Rational Drug Design

The JAK3 structure coordinates or the three-dimensional graphical representation generated from these coordinates may be used in conjunction with a computer for a variety of purposes, including drug discovery.

For example, the structure encoded by the data may be computationally evaluated for its ability to associate with chemical entities. Chemical entities that associate with JAK3 may inhibit or activate JAK3 or its homologues, and are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical three-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

In one embodiment, the invention provides for a method of using a computer for selecting an orientation of a chemical entity that interacts favorably with a binding pocket or domain comprising the steps of:

(a) providing the structure coordinates of said binding pocket or domain on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket or domain;

(c) quantifying the association between said chemical entity and all or part of the binding pocket or domain for different orientations of the chemical entity; and

(d) selecting the orientation of the chemical entity with the most favorable interaction based on said quantified association.

In one embodiment, the docking is facilitated by said quantified association.

In one embodiment, the above method further comprises the following steps before step (a):

(e) producing a crystal of a molecule or molecular complex comprising JAK3 kinase domain or homologue thereof;

(f) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal; and

(g) identifying all or part of a binding pocket that corresponds to said binding pocket.

Three-dimensional structural information in step (a) may be generated by instructions such as a computer program or commands that can generate a three-dimensional representation; subtract distances between atoms; calculate chemical energies for a JAK3 molecule, molecular complex or homologues thereof; or calculate or minimize the chemical energies of an association of JAK3 molecule, molecular complex or homologues thereof to a chemical entity. These types of computer programs are known in the art. The graphical representation can be generated or displayed by commercially available software programs. Examples of software programs include but are not limited to QUANTA (Accelrys, San Diego, Calif. ©2001, 2002), O (Jones et al., *Acta Crystallogr. A*47: 110-119 (1991)) and RIBBONS (Carson, *J. Appl. Crystallogr.* 24: 958-961 (1991)), which are incorporated herein by reference. Certain software programs may imbue this representation with physico-chemical attributes which are known from the chemical composition of the molecule, such as residue charge, hydrophobicity, torsional and rotational degrees of freedom for the residue or segment, etc. Examples of software programs for calculating chemical energies are described below.

The above method may further comprise the following step after step (d): outputting said quantified association to a suitable output hardware, such as a CRT display terminal, a CD or DVD recorder, ZIP™ or JAZ™ drive, a disk drive, or other machine-readable data storage device, as described previously. The method may further comprise generating a three-dimensional structure, graphical representation thereof, or both, of the molecule or molecular complex prior to step (b).

One embodiment of this invention provides for the above method, wherein energy minimization, molecular dynamics simulations, or rigid body minimizations are performed simultaneously with or following step (b).

The above method may further comprise the steps of:

(e) repeating steps (b) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that interacts more favorably with said binding pocket or domain based on said quantified association of said first or second chemical entity.

In another embodiment, the invention provides for the method of using a computer for selecting an orientation of a chemical entity with a favorable shape complementarity in a binding pocket comprising the steps of:

(a) providing the structure coordinates of said binding pocket and all or part of the ligand bound therein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket;

(c) quantitating the contact score of said chemical entity in different orientations; and

(d) selecting an orientation with the highest contact score.

In one embodiment, the docking is facilitated by the contact score.

The method above may further comprise the step of generating a three-dimensional graphical representation of the binding pocket and all or part of the ligand bound therein prior to step (b).

The method above may further comprise the steps of:

(e) repeating steps (b) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that has a higher contact score based on said quantitated contact score of said first or second chemical entity.

In another embodiment, the invention provides a method for screening a plurality of chemical entities to associate at a deformation energy of binding of less than −7 kcal/mol with said binding pocket;

(a) employing computational means, which utilize said structure coordinates to dock one of said plurality of chemical entities in said binding pocket;

(b) quantifying the deformation energy of binding between the chemical entity and the binding pocket;

(c) repeating steps (a) and (b) for each remaining chemical entity; and

(d) outputting a set of chemical entities that associate with the binding pocket at a deformation energy of binding of less than −7 kcal/mol to a suitable output hardware.

In another embodiment, the method comprises the steps of:

(a) constructing a computer model of the binding pocket of said molecule or molecular complex;

(b) selecting a chemical entity to be evaluated by a method selected from the group consisting of assembling said chemical entity; selecting a chemical entity from a small molecule database; de novo ligand design of said chemical entity; and modifying a known agonist or inhibitor, or a portion thereof, of a JAK3 kinase domain, or homologue thereof;

(c) employing computational means to dock said chemical entity to be evaluated in said binding pocket in order to provide an energy-minimized configuration of said chemical entity in the binding pocket; and

(d) evaluating the results of said docking to quantify the association between said chemical entity and the binding pocket.

Alternatively, the structure coordinates of the JAK3 binding pocket may be utilized in a method for identifying a candidate inhibitor of a molecule or molecular complex comprising a binding pocket of JAK3. This method comprises the steps of:

(a) using a three-dimensional structure of the binding pocket or domain to design, select or optimize a plurality of chemical entities;

(b) contacting each chemical entity with the molecule said molecular complex;

(c) monitoring the inhibition to the catalytic activity of the molecule or molecular complex by the chemical entity; and

(d) selecting a chemical entity based on the effect of the chemical entity on the activity of the molecule or molecular complex.

In one embodiment, the three-dimensional structure is displayed as a graphical representation.

In another embodiment, the method comprises the steps of:

(a) constructing a computer model of a binding pocket of the molecule or molecular complex;

(b) selecting a chemical entity to be evaluated by a method selected from the group consisting of assembling said chemical entity; selecting a chemical entity from a small molecule database; de novo ligand design of said chemical entity; and modifying a known agonist or inhibitor, or a portion thereof, of a JAK3 kinase domain or homologue thereof;

(c) employing computation means to dock said chemical entity to be evaluated and said binding pocket in order to provide an energy-minimized configuration of said chemical entity in the binding pocket; and

(d) evaluating the results of said docking to quantify the association between said chemical entity and the binding pocket;

(e) synthesizing said chemical entity; and

(f) contacting said chemical entity with said molecule or molecular complex to determine the ability of said chemical entity to activate or inhibit said molecule.

In one embodiment, the invention provides a method of designing a compound or complex that associates with all or part of the binding pocket comprising the steps of:

(a) providing the structure coordinates of said binding pocket or domain on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) using the computer to dock a first chemical entity in part of the binding pocket or domain;

(c) docking a second chemical entity in another part of the binding pocket or domain;

(d) quantifying the association between the first and second chemical entity and part of the binding pocket or domain;

(e) repeating steps (b) to (d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity;

(f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to the binding pocket or domain on a computer screen using the three-dimensional graphical representation of the binding pocket or domain and said first and second chemical entity; and

(g) assembling the first and second chemical entity into a compound or complex that interacts with said binding pocket by modeling building.

For the first time, the present invention permits the use of molecular design techniques to identify, select and design

chemical entities, including inhibitory compounds, capable of binding to JAK3 or JAK3-like binding pockets, motifs and domains.

Applicant's elucidation of binding pockets on JAK3 provides the necessary information for designing new chemical entities and compounds that may interact with JAK3 substrate, active site, in whole or in part.

Throughout this section, discussions about the ability of a chemical entity to bind to, interact with or inhibit JAK3 binding pockets refer to features of the entity alone.

The design of compounds that bind to or inhibit JAK3 binding pockets according to this invention generally involves consideration of two factors. First, the chemical entity must be capable of physically and structurally associating with parts or all of the JAK3 binding pockets. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

Second, the chemical entity must be able to assume a conformation that allows it to associate with the JAK3 binding pockets directly. Although certain positions of the chemical entity will not directly participate in these associations, those portions of the chemical entity may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of a chemical entity comprising several chemical entities that directly interact with the JAK3 or JAK3-like binding pockets.

The potential inhibitory or binding effect of a chemical entity on JAK3 binding pockets may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given entity suggests insufficient interaction and association between it and the JAK3 binding pockets, testing of the entity is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to a JAK3 binding pocket. This may be achieved by testing the ability of the molecule to inhibit JAK3 using the assay described in Example 9.

A potential inhibitor of a JAK3 binding pocket may be computationally evaluated by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the JAK3 binding pockets.

One skilled in the art may use one of several methods to screen chemical entities or fragments or moieties thereof for their ability to associate with the binding pockets described herein. This process may begin by visual inspection of, for example, any of the binding pockets on the computer screen based on the JAK3 structure coordinates Table 2 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected chemical entities, or fragments or moieties thereof may then be positioned in a variety of orientations, or docked, within that binding pocket as defined supra. Docking may be accomplished using software such as QUANTA (Accelrys, San Diego, Calif. ©2001, 2002) and Sybyl (Tripos Associates, St. Louis, Mo.), followed by, or performed simultaneously with, energy minimization, rigid-body minimization (Gshwend, supra) and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", *J. Med. Chem.* 28: 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.
2. MCSS (Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method," *Proteins Struct. Funct. Genet.* 11: 29-34 (1991)). MCSS is available from Molecular Simulations, San Diego, Calif.
3. AUTODOCK (Goodsell, et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", *Proteins Struct. Funct. and Genet.* 8: 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.
4. DOCK (Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", *J. Mol. Biol.* 161: 269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable chemical entities or fragments have been selected, they can be assembled into single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of JAK3. This would be followed by manual model building using software such as QUANTA (Accelrys, San Diego, Calif. ©2001, 2002) or Sybyl (Tripos Associates, St. Louis, Mo.).

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in *Molecular Recognition in Chemical and Biological Problems*, S. M. Roberts, Ed., Royal Society of Chemistry, Special Publication No. 78: 182-196 (1989); Lauri, G. and Bartlett, P. A., "CAVEAT: A Program to Facilitate the Design of Organic Molecules", *J. Comp. Aid. Molec. Design* 8: 51-66 (1994)), CAVEAT is available from the University of California, Berkeley, Calif.
2. 3D Database systems such as ISIS (MDL Information Systems, San Leandro, Calif.). This area is reviewed in Martin, Y. C., "3D Database Searching in Drug Design", *J. Med. Chem.* 35: 2145-2154 (1992).
3. HOOK (Eisen et al., "HOOK: A program for Finding Novel Molecular Architectures that Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site", *Proteins Struct. Funct. Genet.* 19: 199-221 (1994)). HOOK is available from Molecular Simulations, San Diego, Calif.

Instead of proceeding to build an inhibitor of a JAK3 binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other JAK3 binding compounds may be designed as a whole or "de novo" using either an empty binding pocket or optionally including some portion(s) of a known inhibitor(s). There are many de novo ligand design methods including:

1. LUDI (Böhm, J.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", *J. Comp. Aid. Molec. Design* 6: 61-78 (1992)). LUDI is available from Molecular Simulations Incorporated, San Diego, Calif.
2. LEGEND (Nishibata et al., *Tetrahedron* 47: 8985-8990 (1991)). LEGEND is available from Molecular Simulations Incorporated, San Diego, Calif.
3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).

4. SPROUT (Gillet et al., "SPROUT: A program for Structure Generation)", *J. Comp. Aid. Molec. Design* 7: 127-153 (1993)). SPROUT is available from the University of Leeds, UK.

Other molecular modeling techniques may also be employed in accordance with this invention (see, e.g., Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, *J. Med. Chem.* 33: 883-894 (1990); see also, Navia, M. A. and Murcko, M. A., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology 2: 202-210 (1992); Balbes et al., "A Perspective of Modern Methods in Computer-Aided Drug Design", in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 5: 337-379 (1994); see also, Guida, W. C., "Software For Structure-Based Drug Design", *Curr. Opin. Struct. Biology* 4: 777-781 (1994)).

Once a chemical entity has boon designed or selected by the above methods, the efficiency with which that entity may bind to any of the above binding, pockets may be tested and optimized by computational evaluation. For example, an effective binding pocket inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient binding pocket inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. Binding pocket inhibitors may interact with the binding pocket in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformation observed when the inhibitor binds to the protein.

A chemical entity designed or selected as binding to any one of the above binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. ©1995); AMBER version 4.1 (P. A. Kollman, University of California at San Francisco, ©1995); QUANT/CHARMM (Accelrys, San Diego, Calif. ©2001, 2002); Insight II/Discover (Molecular Simulations, Inc., San Diego, Calif. ©1998); DelPhi (Molecular Simulations, Inc., San Diego, Calif. ©1998); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach enabled by this invention is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to any of the above binding pocket. In this screening, the quality of fit of such entities to the binding pocket may be judged either by shape complementarity or by estimated interaction energy (Meng et al., *J. Comp. Chem.* 13: 505-524 (1992)).

Another particularly useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a chemical entity by determining and evaluating the three-dimensional structures of successive sets protein/chemical entity complexes.

In iterative drug design, crystals of a series of protein or protein complexes are obtained and then the three-dimensional structures of each crystal is solved. Such an approach provides insight into the associated between the proteins and compounds of each complex. This is accomplished by selecting compounds with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three-dimensional structure of the complex, and comparing the associations between the new protein/compound complex and previously solved protein/compound complexes. By observing how changes in compound affected the protein-compound associations, these associations may be optimized.

In some cases, iterative drug design is carried out by forming successive protein-compound complexes and then crystallizing each new complex. High throughput crystallization assays may be used to find a new crystallization condition or to optimize the original protein crystallization condition for the new complex. Alternatively, a pre-formed protein crystal may be soaked in the presence of an inhibitor, thereby forming a protein/compound complex and obviating the need to crystallize each individual protein/compound complex.

In one embodiment, this invention provides a method for identifying a candidate inhibitor that interacts with a binding site of a Janus Kinase 3 kinase protein or a homologue thereof, comprising the steps of:

(a) obtaining a crystal comprising said human Janus Kinase 3 kinase protein or said homologue thereof, wherein the crystal is characterized with space group $P2_1$ and has unit cell parameters of a=59.98 Å, b=90.19 Å, c=69.00 Å; β=111.5°;

(b) obtaining the structure coordinates of amino acids of the crystal step (a), wherein the structure coordinates are set forth in Table 1;

(c) generating a three-dimensional model of said human Janus Kinase 3 kinase protein or said homologue thereof using the structure coordinates of the amino acids obtained in step (b), a root mean square deviation from backbone atoms of said amino acids of not more than ±2.0 Å;

(d) determining a binding site of said human Janus Kinase 3 kinase protein or said homologue thereof from said three-dimensional model; and

(e) performing computer fitting analysis to identify the candidate inhibitor which interacts with said binding site.

In one embodiment, this method further comprising the step of:

(f) contacting the identified candidate inhibitor with said human Janus Kinase 3 kinase protein or said homologue thereof in order to determine the effect of the inhibitor on human Janus Kinase 3 kinase protein activity.

In another embodiment, the binding site of said human Janus Kinase 3 kinase protein or said homologue thereof determined in step (d) comprises the structure coordinates according to Table 1 of amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989,

Pro990 and Trp 993, wherein the root mean square deviation from the backbone atoms of said amino acids is not more than ±2.0 Å.

In one embodiment, this invention provides for a method of for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the steps of:

(a) obtaining a crystal comprising said human Janus Kinase 3 kinase protein or said homologue thereof, wherein the crystal is characterized with space group $P2_1$ and has unit cell parameters of a=59.98 Å, b=90.19 Å, c=69.00 Å; β=111.5°;

(b) obtaining the structure coordinates of amino acids of the crystal of step (a);

(c) generating a three-dimensional model of said human Janus Kinase 3 kinase protein or said homologue thereof using the structure coordinates of the amino acids generated in step (b), a root mean square deviation from backbone atoms of said amino acids of not more than ±2.0 Å;

(d) determining a binding site of said human Janus Kinase 3 kinase protein or said homologue thereof from said three-dimensional model; and

(e) performing computer fitting analysis to identify the candidate inhibitor which interacts with said binding site.

In one embodiment, this method further comprising the step of:

(f) contacting the identified candidate inhibitor with said human Janus Kinase 3 kinase protein or said homologue thereof in order to determine the effect of the inhibitor on human Janus Kinase 3 kinase protein activity.

In another embodiment, the binding site of said human Janus Kinase 3 kinase protein or said homologue thereof determined in step (d) comprises the structure coordinates according to Table 1 of amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993, wherein the root mean square deviation from the backbone atoms of said amino acids is not more than ±2.0 Å.

In another embodiment, this invention provides a method for identifying a candidate inhibitor that interacts with a binding site of a human Janus Kinase 3 kinase protein or a homologue thereof, comprising the step of determining a binding site said human Janus Kinase 3 kinase protein or the homologue thereof from a three-dimensional model to design or identify the candidate inhibitor which interacts with said binding site.

In another embodiment, the binding site of said human Janus Kinase 3 kinase protein or said homologue thereof determined in step (d) comprises the structure coordinates according to Table 1 of amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993, wherein the root mean square deviation from the backbone atoms of said amino acids is not more than ±2.0 Å.

In one embodiment, this invention provides a method for identifying a candidate inhibitor of a molecule or molecular complex comprising a binding pocket or domain selected from the group consisting of:

(i) a set of amino acid residues which are identical to human Janus Kinase 3 kinase a set of amino acid residues that are identical to human Janus Kinase 3 amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn 832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Lys978, Glu985, Gln988, Ser989, Pro990 and Trp 993, according to Table 1, wherein the root mean square deviation from the backbone atoms of said amino acid residues and said human Janus Kinase 3 kinase amino residues is not greater than about 2.0 Å; and

(ii) a set of amino acid residues that are identical to Janus Kinase 3 kinase amino acid residues according to Table 1, wherein the root mean square deviation between said set of amino acid residues and said human Janus Kinase 3 kinase amino acid residues is not more than about 3.0 Å;

comprising the steps of:

(a) using a three-dimensional structure of the binding pocket or domain to design, select or optimize a plurality of chemical entities; and

(b) selecting said candidate inhibitor based on the inhibitory effect of said chemical entities on a human Janus Kinase 3 kinase protein or a human Janus Kinase 3 kinase protein homologue on the catalytic activity of the molecule or molecular complex.

In another embodiment, this invention provides a method of using a crystal of this invention in an inhibitor screening assay comprising:

(a) selecting a potential inhibitor by performing rational drug design with a three-dimensional structure determined for the crystal, wherein said selecting is performed in conjunction with computer modeling;

(b) contacting the potential inhibitor with a kinase; and

(c) detecting the ability of the potential inhibitor for inhibiting the kinase.

Any of the above methods may be used to design peptide or small molecule mimics of the a ligand which may have inhibitory effects on full-length JAK3 protein or fragments thereof, or on full-length JAK3 protein which is mutated in or fragments of the mutated protein thereof.

Structure Determination of Other Molecules

The structure coordinates set forth in Table 2 can also be used in obtaining structural information about other crystallized molecules or molecular complexes. This may be achieved by any of a number of well-known techniques, including molecular replacement.

According to one embodiment, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine readable data which comprises the Fourier transform of at least a portion of the structure coordinates set forth in Table 2 or homology model thereof, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pat-

tern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

In another embodiment, the invention provides a computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex having an unknown structure, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structure coordinates of JAK3 according to Table 2 or homology model thereof;

(b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex having an unknown structure; and

(c) instructions for performing a Fourier transform of the machine-readable data of (a) and for processing said machine-readable data of (b) into structure coordinates.

For example, the Fourier transform of at least a portion of the structure coordinates set forth in Table 2 or homology model thereof may be used to determine at least a portion of the structure coordinates of the molecule or molecular complex.

Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex of unknown structure wherein the molecule or molecular complex is sufficiently homologous to JAK3 kinase domain, comprising the steps of:

(a) crystallizing said molecule or molecular complex of unknown structure;

(b) generating X-ray diffractions data from said crystallized molecule or molecular complex;

(c) applying at least a portion of the JAK3 structure coordinates set forth in one of Table 2 or a homology model thereof to the X-ray diffraction data to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown; and

(d) generating a structural model of the model or molecular complex from the three-dimensional electron density map.

In one embodiment, the methods is performed using a computer. In another embodiment, the molecule is selected from the group consisting of JAK3 kinase domain and a JAK3 kinase domain homologue. In another embodiment, the molecular complex is a JAK3 kinase domain complex or a JAK3 kinase domain homologue complex.

By using molecular replacement, all or part of the structure coordinates of JAK3 as provided by this invention (and set forth in Table 2) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information ab initio.

Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure may provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of JAK3 kinase domain according to Table 2 within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex (E. Lattman, "Use of the Rotation and Translation Functions", in *Meth. Enzymol.* 115: 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser. No. 13, Gordon & Breach, New York (1972)).

The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of the structure of human JAK3 kinase domain can be resolved by this method.

In one embodiment, the method of molecular replacement is utilized to obtain structural information about a JAK3 homologue. The structure coordinates of JAK3 as provided by this invention are particularly useful in solving the structure of JAK3 complexes that are bound by ligands, substrates and inhibitors.

Furthermore, the structure coordinates of JAK3 kinase domain as provided by this invention are useful in solving the structure of JAK3 kinase domains that have amino acid substitutions, additions and/or deletions (referred to collectively as "JAK3 mutants", as compared to naturally occurring JAK3). These JAK3 mutants may optionally be crystallized in co-complex with a chemical entity. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type JAK3. Potential sites for modification within the various binding pockets of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between JAK3 and a chemical entity or compound.

The structure coordinates are also particularly useful in solving the structure of crystals of the kinase domain of JAK3 or homologues co-complexes with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including candidate JAK3 inhibitors. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their JAK3 inhibition activity.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined using 1.5-3.4 Å resolution X-ray data to an R value of about 0.30 or less using computer software, such as X-PLOR (Yale University, ©1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, supra; *Meth. Enzymol. vol.* 114 & 115, H. W. Wyckoff et al., eds. Academic Press (1985)) or CNS (Brunger et al., *Acta Cryst. D*54: 905-921, (1998)).

In order that this invention be more fully understood, the following examples are set forth. These examples are for the purpose of illustration only and are not to be construed as limiting the scope of the invention in any way.

Example 1

Cloning and Expression of JAK3

The full-length JAK3 cDNA (GenBank accession number AAD22741) was obtained by RT-PCR from human bone marrow mRNA (Clontech). A kinase domain JAK3 (A810-E1115) was cloned by PCR from the previously isolated full-length JAK3 cDNA. The PCR product of the kinase domain was cloned into the baculoviral transfer vector pBEV10 for insect cell expression. The recombinant virus was plaque purified and amplified to obtain a high-titer clonal viral stock. For production, High-5 insect cells were grown to 2×10^6 cells/ml in Excell-405 medium (JRH Bioscience, Kans., US) and infected with virus at a multiplicity of infection of 2.5 and incubated for 72-96 hours at 27° C.

Using the same procedure above, the following kinase domains of human JAK3 were also cloned and expressed: amino acid residues 810-1124, amino acid residues 810-1104, and amino acid residues 810-1100.

Example 2

Purification of JAK3

Frozen cell paste was thawed in 5 volumes of Buffer A (50 mM Hepes at pH 8.0, 500 mM NaCl, 20% (v/v) glycerol, 0.2% (v/v) Tween 20, 0.05% (v/v) mM β-mercaptoethanol, 5 mM imidazole, 1 mM PMSF, 5 μg/ml leupeptin, 3 mM benzamidine, and 25 μl/L Benzonase (Novagen, Madison, Wis.) and mechanically lysed in a microfluidizer (Microfluidics, Newton, Mass.). The lysate was centrifuged at 54,000×g for 1 hour, and the supernatant incubated with Talon metal affinity resin (Clonetech, Palo Alto, Calif.) overnight at 4° C. After extensive washing with 20 column volumes of Buffer A, the kinase domain was eluted with Buffer A containing 100 mM imidazole with the pH readjusted to 8.0.

The elution pool was concentrated by ultrafiltration (30 KDa MWCO) in an Amicon stirred cell concentrator (Millipore, Billerica, Mass.) and loaded onto a HR 16/60 Superdex-200 size-exclusion column (Amersham Biosciences, Uppsala, Sweden) equilibrated in Buffer B (50 mM Hepes at pH 8.0, 500 mM NaCl, 20% (v/v) glycerol, 5 mM DTT, and 0.05% (w/v) β-octylglucopyranoside). The JAK3 kinase domain was pooled based on SDS-PAGE analysis and $MgCl_2$ was added to give a final concentration of 20 mM $MgCl_2$.

The JAK3 kinase domain was loaded onto a γ-phenyl ATP-Sepharose column (Haystead et al., *Eur. J. Biochem.* 214: 459-467 (1993)) pre-equilibrated with Buffer C (50 mM Hepes at pH 8.0, 20% (v/v) glycerol, 0.5 M NaCl, 20 mM $MgCl_2$, 0.05% β-octylglucopyranoside, and 5 mM DTT). After washing with two column volumes of Buffer C, JAK3 kinase domain was eluted from the column with 10 mM ADP in Buffer C and the fractions containing JAK3 kinase domain were pooled based on SDS-PAGE analysis.

The hexahistidine tag was cleaved by incubating the protein with 4 units/ml thrombin (Calbiochem, La Jolla, Calif.) at room temperature for two hours. The completion of the cleavage was confirmed by SDS-PAGE and thrombin was removed by treating the protein with benzamidine Sepharose™ 6B (Amersham Biosciences, Uppsala, Sweden) for 30 minutes at room temperature.

The buffer was exchanged to Buffer B using a HR 16/60 Superdex-200 size exclusion column (Amersham Biosciences, Uppsala, Sweden). The kinase domain containing fractions were pooled and concentrated to 15 mg/ml using a 10 KDa MWCO Vivaspin concentrator (Vivascience, Hanover, Germany) in the presence of 2 mM AMP-PNP (ANP) and 4 mM $MgCl_2$. Samples were subjected to ultracentrifugation at 90,000×g for 10 minutes prior to freezing for storage at −80° C.

Example 3

Crystallization of JAK3-Adenosine Complex

The concentrated protein stored at −80° C. from Example 2 above was thawed on ice and centrifuged in a microcentrifuge for 5 minutes prior to crystallization. The protein (10-15 mg/mL in 50 mM Hepes at pH 8.0, 500 mM NaCl, 20% (v/v) glycerol, 5 mM DTT, and 0.05% (w/v) β-octylglucopyranoside) was crystallized by the vapor diffusion method in sitting drop or hanging drop plates using 20-26% PEG 3350 as the precipitant, 200-260 mM KCl, 20 mM spermine, 10 mM DTT and 100 mM bis-tris pH 6.0. Equal volumes of protein and reservoir solution (0.5 μL) were used to form drops. Bigger drops would also grow from 1.0 μL of protein and 1.0 μL of reservoir solution. Crystals usually grew overnight as extremely thin (150×50×<10 μm) highly malleable plates.

Crystals were grown in the Corning® 384 Well plate (available from Fisher Scientific), Greiner crystallization low profile plates (available from Hampton Research (Aliso Viejo, Calif.)), both the 96-well CrystalQuick™ standard profile round and flat bottom plates (available from Hampton Research (Aliso Viejo, Calif.)), and the 24 well VDX plates (available from Hampton Research Aliso Viejo, Calif.)). The volume of the reservoir for the 384-well plate was 50 μL. The volume of the reservoir for the 96-well low profile plate was 100 μL, and for the CrystalQuick™ plates, it was varied between 70-100 μL.

Crystals were obtained for JAK3 protein constructs comprising amino acid residues 810-1100, amino acid residues 810-1104, amino acid residues 810-1115 and amino acid residues 810-1124.

Example 4

X-Ray Data Collection and Structure Determination

Data was collected from crystals of the protein constructs comprising amino acid residues 810-1115 and 810-1124. The details described below, which generated the final data sets used to solve the structure of human JAK3 kinase domain, are for the protein construct comprising amino acid residues 810-1115.

Cryosolvent (reservoir solution containing 25% glycerol) was slowly mixed with the protein drop until no further mixing was observed. The crystals were mounted in nylon loops and flash frozen directly in the nitrogen stream and then stored in liquid nitrogen until the time of data collection. Flash freezing in the nitrogen stream caused less damage to the crystals than freezing directly into liquid nitrogen. The crystals diffracted to greater than 2.1 Å resolution, but the spot shape was distorted at higher than 2.5 Å resolution, and the data suffered from severe anisotropy. Therefore, although the crystals diffracted to greater than 2.1 Å, data were only useable to 2.5 Å.

The data were collected at the beamline 5.0.2 at the Advanced Light Source (ALS) Berkeley, Calif. using 1.0 Å

X-rays and an ADSC CCD detector. The data from the crystal were integrated and scaled using d*TREK (Pflugrath, *Acta Crystallogr.* D55: 1718-1725 (1999)). Structure factors were calculated using TRUNCATE (Bailey, *Acta Crystallogr.* D50: 760-763). Table 1 summarizes data collection.

The crystal belonged to spacegroup $P2_1$ with unit cell dimensions a=59.98 Å, b=90.19 Å, c=69.00 Å, α=90°, β=111.5°, γ=90° with 2 molecules in the asymmetric unit. A second crystal form that belonged to spacegroup $P2_12_12_1$ with unit cell dimensions a=72.36 Å, b=90.04 Å, c=105.60 Å, α=β=γ=90° also formed. The discussions below will be limited to the crystals belonging to the $P2_1$ spacegroup.

The orientation and position of JAK3 within the asymmetric unit was achieved by molecular replacement using BEAST (Read, *Acta Crystallogr. D*547: 1373-1382 (2001)). BEAST uses maximum likelihood targets for the rotation and translation functions, and allows the use of multiple models, allowing the creation of a statically-weighted set of averaged structure factors. The use of BEAST was essential in solving the structure. Protein kinases are very flexible molecules in their inactive state (Huse and Kuriyan, *Cell* 109: pp. 275-282 (20002)). While conventional molecular replacement methods failed, BEAST, which uses maximum likelihood targets for the rotation and translation functions, allowed the use of multiple models, and created from these models a statistically-weighted set of averaged structure factors.

Multiple superimposed kinase domains with the activation loop removed were used as the search model (Protein Data Bank (PDB) accession codes 1M17, 1LUF, 1FVR, 1IEP, 1JPA, 1AGW, 1IR3, 1QPC, and 1GJO). The superposition of the structures was done using the program DeepView (Guex and Peitsch, *Electrophoresis* 18: 2714-2723). The initial set of structures chosen represented molecules with high sequence homology to JAK3, and were in a variety of conformations. The BEAST rotation function yielded two distinct peaks, which were related by the observed non-crystallographic symmetric. Of the kinase domains used, epidermal grown factor receptor (1M17), had the highest sequence homology to JAK3, therefore, EGFR was used as the initial model for rigid body refinement in CNX (Accelrys, San Diego, Calif.).

Initial calculated electron density maps revealed that the C-terminal domain was positioned correctly, but the N-terminal domain was not. In order to find the proper orientation of the N-terminal domain, several hybrid molecules were created. The C-terminal domain of another tyrosine kinase was superimposed onto the C-terminal domain of EGFR. The new molecule used for rigid body refinement consisted of the C-terminal domain of EGFR and the newly positioned N-terminal domain of the other kinase. Of the hybrid kinases created, the molecule with the N-terminal domain of src kinase (PDB accession code 2SRC) and the C-terminal domain of EGFR yielded an easily interpretable electron density map in both domains.

The position of the ANP ligand could be clearly seen in the initial electron density maps. The structure was refined using CNX (Accelrys, San Diego, Calif.). Initial rigid-body refinement of the hybrid Src-EGFR kinase domain was followed by mutation of the necessary side chains in order to reflect the human JAK3 sequence, and proper placement of those side chains into the initial electron density maps. Subsequent refinement consisted of rounds of energy minimization, simulated annealing, and B factor refinement using NCS restraints, which were alternated with manual rebuilding of the structure in QUANTA (Accelrys, San Diego, Calif. ©2001, 2002).

Table 1 summarizes refinement statistics. Poor electron density was observed for the extreme N-terminus of the molecule (residues 810-812) and no electron density was observed for the extreme C-terminus (residues 1102-1115). A glycerol molecule was modeled into unaccounted electron density near the surface of the molecule. The final refined structure model includes human JAK3 kinase amino acid residues 813-1100 of SEQ ID NO:1.

The asymmetric unit contains two molecules of human JAK3 (labeled as mol A and B in FIG. **1**). The overall RMSD for 288 Cα atoms between the two structures is 0.20 Å, and the overall RMSSD for 1152 backbone atoms is 0.23 Å. Throughout the refinement non-crystallographic restraints were used. The largest area of difference between the two molecules is the activation loop. If Molecule B is the fixed molecule and Molecule A is the moving molecule, then the relationship between A and B is the following:

ROTATION MATRIX:	−0.54749	−0.00940	0.83676
	0.00861	−0.99995	−0.00560
	0.83677	0.00414	0.54754
TRANSLATION VECTOR IN AS	4.32576	73.98868	6.79225

The overall R-factor and R_{free} of the final model were 24.5% and 31.1%, respectively. The test set was composed of 7.9% of the total reflections.

Table 2 lists the atomic structure coordinates in Protein Data Bank (PDB)-like format and header for human JAK3 in complex with AMP-PNP (JAK3-AMP-PNP complex), as derived by X-ray diffraction from a crystal of the complex. The structure model includes human JAK3 kinase amino acid residues 813-1100 of SEQ ID NO:1).

The following abbreviations are used in Table 2:

"Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.

"Resid" refers to the amino acid residue in the molecular model.

"X, Y, Z" define the atomic position of the element measured.

"B" is a thermal factor that measures movement of the atom around its atomic center.

"Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in the molecules.

"Mol" refers to a molecule in the asymmetric unit. Mol A and Mol B are JAK3 protein molecules. Mol Y and Mol Z are AMP-PNP. Mol Y and Mol Z binds to Mol A and Mol B of JAK3 protein, respectively. Mol W is water.

Residue "AMP" represents AMP-PNP.

Example 8

Overview of Crystal Structure of JAK3-AMP-PNP Complex

FIG. **1** shows the overall fold of the JAK3 kinase domain. The overall structure of the unactivated JAK3 kinase domain is similar to the typical kinase-fold found in both serine-threonine and tyrosine kinases. The protein structure is composed of two domains connected by a flexible linker or hinge (residues 898-905). The smaller N-terminal domain is mostly β-sheet structure (β1-β5), with the exception of a predominant helix, called the αC helix. The C-terminal domain is

composed of two β-strands (β and β8) and seven conserved helices (αD, αE, αEF, and αF-αI), which are found in all protein kinases. However, the JAK3 C-terminal domain also contains structural insertions including an extra helix between αF and αG, referred to herein as αFG.

The JAK3 C-terminal domain region between αF and αG contains a total of three structural insertions when compared to other tyrosine kinases. The first insertion (I1) is between amino acid residues 1024 and 1029. Here the chain juts out away from the C-terminal domain as compared to that of other tyrosine kinases. The structure briefly returns to register with other tyrosine kinases at P1030. The second structural insertion is the short αFG helix (1030-1038). In the αFG helix the side chain of amino acid residue F1034 is in the approximate position of the phenyl ring of a conserved tyrosine found in other tyrosine kinases. The final insertion (I3), amino acid residues 1039-1046, like I1, extends away from The C-terminal domain.

Comparisons of Structures of JAK3-Inhibitor Complexes to Structures of Other Kinases

Comparison of the JAK3 with other protein kinases reveals that the overall orientation of the N- and C-terminal domains is related to that of the Src-2 structure (Xu et al., *Mol. Cell* 3: pp. 629-638 (1999)). The root mean square deviation between Src-2 and JAK3 using 260 equivalent Cα positions is 3.4 Å. Both structures are in an inactive conformation. Like Src-2 and the unactivated CDK2/ATP structure (Schulze-Gahmen et al., *J. Med. Chem.* 39: pp. 4540-4546 (1996)), the position of the C-helix results in a nonproductive alignment of the AMP-PNP phosphate groups. The major difference in the overall architecture of the JAK3 structure and the structures of the inactive forms of Src-2 and CDK2/ATP is the αFG helix region and the conformation of the activation loop. In addition, CDK2 is a Serine/Threonine kinase, not a Tyrosine kinase as are Src-2 and JAK3, and as such it has a large insertion region between the G and H helices.

While the N-terminus of the activation loop of JAK3 is similar to that of Src-2 structure, the C-terminus of the activation loop is kinked similar to the activation loops of the FGF-1 receptor/ACP and CDK2/ATP complex structures. This kink effectively blocks the peptide substrate site. In the FGF-1 receptor, although the C-terminus of the activation loop is kinked, the overall structure is in a more open conformation and the activation loop does not reach the glycine-rich loop. However, in the unactivated CDK2/ATP structure, the activation loops does interact with the glycine-rich loop (Schulze-Gahmen et al., *J. Med. Chem.* 39: pp. 4540-4546 (1996)). In JAK3, N832 of the glycine-rich loop makes two hydrogen bonds to the activation loop. The main chain carbonyl group is hydrogen bonded to the Nζ group of K978 and the Nδ of the side chain is hydrogen bonded to the main chain carbonyl group of E988. The interaction network also includes the γ-phosphate of the ATP analogue.

The active site, which contains the non-hydrolyzable ATP analogue, AMP-PNP, is formed by a groove at the interface between the N and C-terminal lobes. The hinge region, the glycine rich loop (residues 829-834), and the activation loop (residues 967-990) enclose the ligand. The NH2 of the purine ring is hydrogen bonded to the backbone oxygen of Glu 903 (FIG. **6**). The phosphates of the AMP-PNP participate in an extensive hydrogen bonding network that includes both the activation and glycine-rich loops (FIG. **6**).

The orientation of the N and C-terminal lobes of Jak3 KD1 structure is most similar to that of the unactivated Src kinase (Xu, W., Doshi, A., Lei, M., Eck, M. J. and Harrison, S. C. (1999) *Mol Cell* 3, 629-638), Cdk-2 (Schulze Gahmen, U. Brandsen, J., Jones, H. D., Morgan, D. O. Meijer, L., Vesely, J., and Kim, S. H. (1995) *Proteins* 22, 378-391), and the recently solved structures of Mek1 and Mek2 (Ohren, J. F., Chen, H., Pavlovsky, A., Whitehead, C., Zhang, E., Kuffa, P., Yan, C., McConnell, P., Spessard, C., Banotai, C., Mueller, W. T., Delaney, A., Omer, C., Sebolt-Leopold, J. Dudley, D. T., Leung, I. K. Flamme, C., Warmus J., Kaufman, M., Barrett, S., Tecle, H., and Hasemann, C. A. (2004) *Nat Struct Mol Biol* 11, 1192-1197). The root mean square deviation (r.m.s.d.) between Jak3 and the Src-2, Cdk-2, Mek-1, and Mek-2 structures is 1.15 Å (using 215 equivalent Cα positions), 1.36 Å (using 186 equivalent Cα positions), 1.56 Å (using 190 equivalent Cα positions), and 1.63 Å (using 191 equivalent Cα positions) respectively. As in the previously mentioned structures, the αC-helix which contains the conserved glutamic acid, Glu 871, is swung out, away from the active site preventing the formation of the salt bridge between Glu 871 and the conserved catalytic lysine, Lys 855, which in activated kinases coordinates the α and β phosphates of the ATP. Instead Lys 855 is hydrogen bonded to the α-phosphate of the AMP-PNP, and the aspartic acid, Asp 967, at the beginning of the activation loop. The conformation of the AMP-PNP, the coordination of the Mg^{2+} ion, and the interaction with the catalytic lysine, Lys 855, are all very similar to that seen in the inactive Cdk-2/ATP (Schulze Gahmen, U., De Bondt, H. L., and Kim, S. H. (1996) *J Med Chem* 39, 4540-4546) and Src-2 structures (Xu, W. Doshi, A., Lei, M., Eck, M. J., and Harrison, S. C. (1999) *Mol Cell* 3, 629-638).

The beginning of the activation loop, containing the conserved DFG sequence (residues 967-968), is almost identical in conformation to that in the Src-2 and unactivated Cdk-2 structures. However, the Jak3 KD1 activation loop notably diverges from the previously mentioned structures, Src-2 and Cdk-2, as it kinks toward the glycine-rich loop. Superposition of Jak3 on insulin receptor kinase with a bound peptide substrate (PDB #IIR3) clearly showed the kink in the activation loop (residues 978-989) blocks the protein substrate binding site, similar to that seen in unactivated Cdk-2 (PDB #1HCK) (Schulze-Gahmen, U., De Bondt, H. L., and Kim, S. H. (1996) *J Med Chem* 39, 4540-4546) and fibroblast growth factor receptor kinase (PDB #1FGK (Mohammadi, M., Schlessinger, J., and Hubbard, S. R. (1996) *Cell* 86, 577-587). This region of the activation loop includes the potential autophosphorylation tyrosines, Tyr 980 and Tyr 981.

Regulation of the Catalytic Domain of JAK3

Regulation of the catalytic domain of Janus kinases takes place through interactions with domains N-terminal to the kinase domain. Both the pseudokinase domain and the FERM domain play pivotal roles in controlling activity of the catalytic domain. Furthermore, it has been shown that both of these domains can interact with the kinase domain. Previous studies in JAK3 have focused on naturally occurring mutations in the FERM domain and pseudokinase domain that have been found in SCID patients. Unique region around αFG is a possible site for interaction with the other JAK3 domains.

Some known SCID mutations affect the kinase domain. There are two known SCID mutations that prematurely terminate the kinase domain. These premature stops remove the αFG-α1 helices. These prematurely terminated kinases probably result in an unstable kinase domain, which may be rapidly degraded in cells. This would explain the undetectable levels of protein expressed in cells containing these mutations. The only naturally occurring point mutation in the catalytic domain resulting in SCID known is the mutation of a leucine at position 910 (L910) to serine. L910 occurs at the beginning of the αD helix. The side chain of L910 contributes to the hydrophobic core of the C-terminal domain. This resi-

due is only five residues away from L905, which is involved in positioning the purine ring of the ATP substrate, and one residue away from R911, R918, have been implicated in binding the peptide substrate at the P-1, P-2 and P-3 positions. The replacement of a highly conserved hydrophobic residue, leucine, with a polar residue, serine, may result in the disruption or distortion of the αD helix, which may affect the binding of either the ATP substrate and/or the peptide substrate.

The invention between αF and αG appears to be a unique feature of the JAK family when compared to the same region in other receptor and non-receptor tyrosine kinases. This insertion structurally encompasses a rather large region on the surface of the kinase domain as compared to other kinases, such as c-scr. The αFG insertion region creates a large potential binding surface for recognition by another domain of the JAK kinases, specifically, the N-terminal FERM domain or the pseudokinase domain or perhaps another protein. In fact, it has been suggested that messages in other domains affect the function of the kinase domain. This region may be docking site for either another domain within the JAK kinase or for an exogenous protein substrate.

Example 9

Activity Assay

To each well of a 96-well polycarbonate plate is added 1.5 μL of a candidate JAK3 inhibitor along with 50 μL of kinase buffer (100 mM Hepes at pH 7.4, 1 mM DTT, 10 mM $MgCl_2$, 25 mM NaCl and 0.01% BSA) containing 2 uM poly$(Glu)_4$Tyr and 10 μM ATP. This is then mixed and 50 μL of kinase buffer containing 2 nM JAK3 enzyme is added to start the reaction. After 20 minutes at room temperature (25° C.), the reaction is stopped with 50 μL of 20% trichloroacetic acid (TCA) that also contains 0.4 mM ATP. The entire contents of each well is then transferred to a 96-well glass fiber filter plate using a TomTek Cell Harvester. After washing, 60 μL of scintillation fluid is added and ^{33}P incorporated is detected on a Perkin Elmer® TopCount instrument.

JAK2 activity can be assayed as above, except that final poly$(Glu)_4$Tyr concentration is 15 μM and final ATP concentration is 12 μM.

While we have described a number of embodiments of this invention, it is apparent that our basic constructions may be altered to provide other embodiments which utilize the products, processes and methods of this invention.

TABLE 1

Data Collection and Refinement Statistics	
Data set	AMP-PNP
Data collection	
X-ray source	ALS 5.0.2
Space group	$P2_1$
Unit cell parameters (Å)	a = 59.98 Å, b = 90.19 Å, c = 69.00 Å, β = 111.5°
Resolution (Å)	45.54-2.50 (2.59-2.50)
Unique reflections	23427
Redundancy	3.23 (3.12)
Completeness (%)*	98.6 (94.2)
R_{merge}*	0.124 (0.393)
<I/σ>*	5.4 (2.2)
Refinement	
Reflections used	22832
Test reflections	1806
R-factor	24.5% (28.5%)
Free R-factor (% data)	31.1% (36.1%)
RMS deviation	
Bond lengths (Å)	0.009
Bond angles (°)	1.4
Dihedral angles (°)	22.4
Protein atoms	4612
Solvent atoms	176

*Values for the highest resolution shell are shown in parentheses, $R_{merge} = \Sigma_{hkl} \Sigma_i |I(hkl)_i - \langle I(hkl) \rangle| / \Sigma_{hkl} \Sigma_i \langle I(hkl)_i \rangle$ over i observations of reflection hkl.

R-factor = $\Sigma ||F_{obs}| - |F_{calc}|| / \Sigma |F_{obs}|$ where F_{obs} and F_{calc} are the observed and calculated structure factors, respectively. Free R-factor is calculated from a randomly chosen subset of reflections not used for refinement.

TABLE 2

```
REMARK
REMARK   3  REFINEMENT.
REMARK   3    PROGRAM         : CNX 2002
REMARK   3    AUTHORS         : Brunger, Adams, Clore, Delano,
REMARK   3                      Gros, Grosse-Kunstleve, Jiang,
REMARK   3                      Kuszewski, Nilges, Pannu, Read,
REMARK   3                      Rice, Simonson, Warren
REMARK   3                    And
REMARK   3                  Accelrys Inc.,
REMARK   3                      (Badger, Berard, Kumar, Szalma,
REMARK   3                    Yip, Dzakula).
REMARK   3
REMARK   3   DATA USED IN REFINEMENT.
REMARK   3    RESOLUTION RANGE HIGH       (ANGSTROMS) : 2.50
REMARK   3    RESOLUTION RANGE LOW        (ANGSTROMS) :  19.83
REMARK   3    DATA CUTOFF                   (SIGMA(F)) : 1.0
REMARK   3    DATA CUTOFF HIGH                (ABS(F)) :  1153422.38
REMARK   3    DATA CUTOFF LOW                 (ABS(F)) :    0.000000
REMARK   3    COMPLETENESS (WORKING + TEST)        (%) : 96.2
REMARK   3    NUMBER OF REFLECTIONS                    : 22832
REMARK   3
REMARK   3   FIT TO DATA USED IN REFINEMENT.
REMARK   3    CROSS-VALIDATION METHOD                  : THROUGHOUT
REMARK   3    FREE R VALUE TEST SET SELECTION          : RANDOM
REMARK   3    R VALUE                  (WORKING SET) : 0.245
REMARK   3    FREE R VALUE                           : 0.311
```

TABLE 2-continued

```
REMARK   3   FREE R VALUE TEST SET SIZE                (%) :  7.9
REMARK   3   FREE R VALUE TEST SET COUNT                  :  1806
REMARK   3   ESTIMATED ERROR OF FREE R VALUE              : 0.007
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED                    :  6
REMARK   3   BIN RESOLUTION RANGE HIGH                (A) : 2.50
REMARK   3   BIN RESOLUTION RANGE LOW                 (A) : 2.66
REMARK   3   BIN COMPLETENESS (WORKING + TEST)        (%) : 94.7
REMARK   3   REFLECTIONS IN BIN              (WORKING SET) :  3423
REMARK   3   BIN R VALUE                     (WORKING SET) : 0.285
REMARK   3   BIN FREE R VALUE                              : 0.361
REMARK   3   BIN FREE R VALUE TEST SET SIZE           (%) :  7.7
REMARK   3   BIN FREE R VALUE TEST SET COUNT              :  286
REMARK   3   ESTIMATED ERROR OF BIN FREE R VALUE          : 0.021
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 4612
REMARK   3   NUCLEIC ACID ATOMS       :    0
REMARK   3   HETEROGEN ATOMS          :   64
REMARK   3   SOLVENT ATOMS            :  176
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT                  (A**2) : 24.1
REMARK   3   MEAN B VALUE           (OVERALL, A**2) : 33.3
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :   5.72
REMARK   3    B22 (A**2) :   0.10
REMARK   3    B33 (A**2) :  -5.81
REMARK   3    B12 (A**2) :   0.00
REMARK   3    B13 (A**2) :  -4.61
REMARK   3    B23 (A**2) :   0.00
REMARK   3
REMARK   3  BULK SOLVENT MODELING.
REMARK   3   METHOD USED   : FLAT MODEL
REMARK   3   KSOL          : 0.398536
REMARK   3   BSOL          : 68.0347 (A**2)
REMARK   3
REMARK   3  ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM LUZZATI PLOT                (A) : 0.34
REMARK   3   ESD FROM SIGMAA                      (A) : 0.35
REMARK   3   LOW RESOLUTION CUTOFF                (A) : 5.00
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT            (A) : 0.45
REMARK   3   ESD FROM C-V SIGMAA                  (A) : 0.42
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS                         (A) : 0.009
REMARK   3   BOND ANGLES                  (DEGREES) : 1.4
REMARK   3   DIHEDRAL ANGLES              (DEGREES) : 22.4
REMARK   3   IMPROPER ANGLES              (DEGREES) : 0.82
REMARK   3
REMARK   3  ISOTROPIC THERMAL MODEL: RESTRAINED
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.      RMS      SIGMA
REMARK   3   MAIN-CHAIN BOND                  (A**2) :  1.38   ;  1.50
REMARK   3   MAIN-CHAIN ANGLE                 (A**2) :  2.29   ;  2.00
REMARK   3   SIDE-CHAIN BOND                  (A**2) :  2.01   ;  2.00
REMARK   3   SIDE-CHAIN ANGLE                 (A**2) :  2.92   ;  2.50
REMARK   3
REMARK   3  NCS MODEL: CONSTR
REMARK   3
REMARK   3  NCS RESTRAINTS.                           RMS    SIGMA/WEIGHT
REMARK   3   GROUP  1  POSITIONAL                (A) : NULL  ; NULL
REMARK   3   GROUP  1  B-FACTOR                  (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1  :
ACCELRYS_CNX: libraries/toppar/protein_rep.param
REMARK   3  PARAMETER FILE  2  :
ACCELRYS_CNX: libraries/toppar/water_rep.param
REMARK   3  PARAMETER FILE  3  : parm/missing.dat
REMARK   3  PARAMETER FILE  4  : parm/parmxray.xpl
REMARK   3  PARAMETER FILE  5  : ACCELRYS_CNX: libraries/toppar/ion.param
REMARK   3  TOPOLOGY FILE  1  :
ACCELRYS_CNX: libraries/toppar/protein.top
REMARK   3  TOPOLOGY FILE  2  : parm/mass1.dat
REMARK   3  TOPOLOGY FILE  3  : ACCELRYS_CNX: libraries/toppar/water.top
REMARK   3  TOPOLOGY FILE  4  : inhib.gol.rtf
REMARK   3  TOPOLOGY FILE  5  : ACCELRYS_CNX: libraries/toppar/ion.top
```

TABLE 2-continued

```
REMARK     3
REMARK     3  OTHER REFINEMENT REMARKS: NULL
SEQRES     1 A     288  ASP  PRO  THR  ILE  PHE  GLU  GLU  ARG  HIS  LEU  LYS  TYR  ILE
SEQRES     2 A     288  SER  GLN  LEU  GLY  LYS  GLY  ASN  PHE  GLY  SER  VAL  GLU  LEU
SEQRES     3 A     288  CYS  ARG  TYR  ASP  PRO  LEU  GLY  ASP  ASN  THR  GLY  ALA  LEU
SEQRES     4 A     288  VAL  ALA  VAL  LYS  GLN  LEU  GLN  HIS  SER  GLY  PRO  ASP  GLN
SEQRES     5 A     288  GLN  ARG  ASP  PHE  GLN  ARG  GLU  ILE  GLN  ILE  LEU  LYS  ALA
SEQRES     6 A     288  LEU  HIS  SER  ASP  PHE  ILE  VAL  LYS  TYR  ARG  GLY  VAL  SER
SEQRES     7 A     288  TYR  GLY  PRO  GLY  ARG  GLN  SER  LEU  ARG  LEU  VAL  MET  GLU
SEQRES     8 A     288  TYR  LEU  PRO  SER  GLY  CYS  LEU  ARG  ASP  PHE  LEU  GLN  ARG
SEQRES     9 A     288  HIS  ARG  ALA  ARG  LEU  ASP  ALA  SER  ARG  LEU  LEU  LEU  TYR
SEQRES    10 A     288  SER  SER  GLN  ILE  CYS  LYS  GLY  MET  GLU  TYR  LEU  GLY  SER
SEQRES    11 A     288  ARG  ARG  CYS  VAL  HIS  ARG  ASP  LEU  ALA  ALA  ARG  ASN  ILE
SEQRES    12 A     288  LEU  VAL  GLU  SER  GLU  ALA  HIS  VAL  LYS  ILE  ALA  ASP  PHE
SEQRES    13 A     288  GLY  LEU  ALA  LYS  LEU  LEU  PRO  LEU  ASP  LYS  ASP  TYR  TYR
SEQRES    14 A     288  VAL  VAL  ARG  GLU  PRO  GLY  GLN  SER  PRO  ILE  PHE  TRP  TYR
SEQRES    15 A     288  ALA  PRO  GLU  SER  LEU  SER  ASP  ASN  ILE  PHE  SER  ARG  GLN
SEQRES    16 A     288  SER  ASP  VAL  TRP  SER  PHE  GLY  VAL  VAL  LEU  TYR  GLU  LEU
SEQRES    17 A     288  PHE  THR  TYR  CYS  ASP  LYS  SER  CYS  SER  PRO  SER  ALA  GLU
SEQRES    18 A     288  PHE  LEU  ARG  MET  MET  GLY  CYS  GLU  ARG  ASP  VAL  PRO  ALA
SEQRES    19 A     288  LEU  CYS  ARG  LEU  LEU  GLU  LEU  LEU  GLU  GLU  GLY  GLN  ARG
SEQRES    20 A     288  LEU  PRO  ALA  PRO  PRO  ALA  CYS  PRO  ALA  GLU  VAL  HIS  GLU
SEQRES    21 A     288  LEU  MET  LYS  LEU  CYS  TRP  ALA  PRO  SER  PRO  GLN  ASP  ARG
SEQRES    22 A     288  PRO  SER  PHE  SER  ALA  LEU  GLY  PRO  GLN  LEU  ASP  MET  LEU
SEQRES    23 A     288  TRP  SER
SEQRES     1 B     288  ASP  PRO  THR  ILE  PHE  GLU  GLU  ARG  HIS  LEU  LYS  TYR  ILE
SEQRES     2 B     288  SER  GLN  LEU  GLY  LYS  GLY  ASN  PHE  GLY  SER  VAL  GLU  LEU
SEQRES     3 B     288  CYS  ARG  TYR  ASP  PRO  LEU  GLY  ASP  ASN  THR  GLY  ALA  LEU
SEQRES     4 B     288  VAL  ALA  VAL  LYS  GLN  LEU  GLN  HIS  SER  GLY  PRO  ASP  GLN
SEQRES     5 B     288  GLN  ARG  ASP  PHE  GLN  ARG  GLU  ILE  GLN  ILE  LEU  LYS  ALA
SEQRES     6 B     288  LEU  HIS  SER  ASP  PHE  ILE  VAL  LYS  TYR  ARG  GLY  VAL  SER
SEQRES     7 B     288  TYR  GLY  PRO  GLY  ARG  GLN  SER  LEU  ARG  LEU  VAL  MET  GLU
SEQRES     8 B     288  TYR  LEU  PRO  SER  GLY  CYS  LEU  ARG  ASP  PHE  LEU  GLN  ARG
SEQRES     9 B     288  HIS  ARG  ALA  ARG  LEU  ASP  ALA  SER  ARG  LEU  LEU  LEU  TYR
SEQRES    10 B     288  SER  SER  GLN  ILE  CYS  LYS  GLY  MET  GLU  TYR  LEU  GLY  SER
SEQRES    11 B     288  ARG  ARG  CYS  VAL  HIS  ARG  ASP  LEU  ALA  ALA  ARG  ASN  ILE
SEQRES    12 B     288  LEU  VAL  GLU  SER  GLU  ALA  HIS  VAL  LYS  ILE  ALA  ASP  PHE
SEQRES    13 B     288  GLY  LEU  ALA  LYS  LEU  LEU  PRO  LEU  ASP  LYS  ASP  TYR  TYR
SEQRES    14 B     288  VAL  VAL  ARG  GLU  PRO  GLY  GLN  SER  PRO  ILE  PHE  TRP  TYR
SEQRES    15 B     288  ALA  PRO  GLU  SER  LEU  SER  ASP  ASN  ILE  PHE  SER  ARG  GLN
SEQRES    16 B     288  SER  ASP  VAL  TRP  SER  PHE  GLY  VAL  VAL  LEU  TYR  GLU  LEU
SEQRES    17 B     288  PHE  THR  TYR  CYS  ASP  LYS  SER  CYS  SER  PRO  SER  ALA  GLU
SEQRES    18 B     288  PHE  LEU  ARG  MET  MET  GLY  CYS  GLU  ARG  ASP  VAL  PRO  ALA
SEQRES    19 B     288  LEU  CYS  ARG  LEU  LEU  GLU  LEU  LEU  GLU  GLU  GLY  GLN  ARG
SEQRES    20 B     288  LEU  PRO  ALA  PRO  PRO  ALA  CYS  PRO  ALA  GLU  VAL  HIS  GLU
SEQRES    21 B     288  LEU  MET  LYS  LEU  CYS  TRP  ALA  PRO  SER  PRO  GLN  ASP  ARG
SEQRES    22 B     288  PRO  SER  PHE  SER  ALA  LEU  GLY  PRO  GLN  LEU  ASP  MET  LEU
SEQRES    23 B     288  TRP  SER
CRYST1   59.979   90.191   68.998  90.00 111.49  90.00 P 21                      4
ORIGX1      1.000000    0.000000    0.000000        0.00000
ORIGX2      0.000000    1.000000    0.000000        0.00000
ORIGX3      0.000000    0.000000    1.000000        0.00000
SCALE1      0.016672    0.000000    0.006563        0.00000
SCALE2      0.000000    0.011088    0.000000        0.00000
SCALE3      0.000000    0.000000    0.015576        0.00000
ATOM      1  CB   ASP  A  813      0.580   50.367  -0.785  1.00  41.79  A  C
ATOM      2  CG   ASP  A  813      1.998   49.832  -0.801  1.00  43.65  A  C
ATOM      3  OD1  ASP  A  813      2.838   50.329  -0.016  1.00  46.37  A  O
ATOM      4  OD2  ASP  A  813      2.273   48.916  -1.599  1.00  42.84  A  O
ATOM      5  C    ASP  A  813      1.327   52.295  -2.160  1.00  40.95  A  C
ATOM      6  O    ASP  A  813      1.392   51.562  -3.146  1.00  42.84  A  O
ATOM      7  N    ASP  A  813     -0.881   52.355  -1.021  1.00  40.53  A  N
ATOM      8  CA   ASP  A  813      0.529   51.886  -0.931  1.00  41.34  A  C
ATOM      9  N    PRO  A  814      1.959   53.476  -2.104  1.00  39.43  A  N
ATOM     10  CD   PRO  A  814      1.808   54.433  -0.997  1.00  38.58  A  C
ATOM     11  CA   PRO  A  814      2.775   54.055  -3.176  1.00  37.23  A  C
ATOM     12  CB   PRO  A  814      3.106   55.453  -2.654  1.00  37.73  A  C
ATOM     13  CG   PRO  A  814      1.992   55.748  -1.708  1.00  39.50  A  C
ATOM     14  C    PRO  A  814      4.044   53.287  -3.480  1.00  35.24  A  C
ATOM     15  O    PRO  A  814      4.660   52.693  -2.598  1.00  34.89  A  O
ATOM     16  N    THR  A  815      4.424   53.332  -4.748  1.00  34.06  A  N
ATOM     17  CA   THR  A  815      5.634   52.702  -5.241  1.00  31.98  A  C
ATOM     18  CB   THR  A  815      5.350   51.911  -6.492  1.00  30.59  A  C
ATOM     19  OG1  THR  A  815      4.429   50.863  -6.172  1.00  30.79  A  O
ATOM     20  CG2  THR  A  815      6.637   51.342  -7.065  1.00  26.89  A  C
ATOM     21  C    THR  A  815      6.534   53.867  -5.604  1.00  32.10  A  C
ATOM     22  O    THR  A  815      7.705   53.702  -5.925  1.00  30.98  A  O
ATOM     23  N    ILE  A  816      5.945   55.054  -5.552  1.00  32.69  A  N
ATOM     24  CA   ILE  A  816      6.628   56.297  -5.858  1.00  33.81  A  C
ATOM     25  CB   ILE  A  816      6.003   56.976  -7.097  1.00  35.98  A  C
```

TABLE 2-continued

ATOM	26	CG2	ILE	A	816	6.212	58.473	−7.038	1.00	36.08	A	C
ATOM	27	CG1	ILE	A	816	6.586	56.359	−8.378	1.00	38.71	A	C
ATOM	28	CD1	ILE	A	816	6.128	54.918	−8.667	1.00	37.14	A	C
ATOM	29	C	ILE	A	816	6.482	57.205	−4.645	1.00	32.03	A	C
ATOM	30	O	ILE	A	816	5.380	57.406	−4.146	1.00	33.36	A	O
ATOM	31	N	PHE	A	817	7.603	57.736	−4.174	1.00	29.99	A	N
ATOM	32	CA	PHE	A	817	7.628	58.601	−3.011	1.00	28.59	A	C
ATOM	33	CB	PHE	A	817	8.362	57.897	−1.863	1.00	28.20	A	C
ATOM	34	CG	PHE	A	817	7.528	56.863	−1.149	1.00	25.21	A	C
ATOM	35	CD1	PHE	A	817	6.790	57.203	−0.033	1.00	25.13	A	C
ATOM	36	CD2	PHE	A	817	7.481	55.556	−1.593	1.00	23.71	A	C
ATOM	37	CE1	PHE	A	817	6.022	56.258	0.630	1.00	22.04	A	C
ATOM	38	CE2	PHE	A	817	6.712	54.609	−0.928	1.00	21.29	A	C
ATOM	39	CZ	PHE	A	817	5.987	54.965	0.181	1.00	19.64	A	C
ATOM	40	C	PHE	A	817	8.303	59.927	−3.324	1.00	28.82	A	C
ATOM	41	O	PHE	A	817	9.451	59.981	−3.778	1.00	27.53	A	O
ATOM	42	N	GLU	A	818	7.575	61.001	−3.064	1.00	29.51	A	N
ATOM	43	CA	GLU	A	818	8.067	62.344	−3.311	1.00	31.25	A	C
ATOM	44	CB	GLU	A	818	6.872	63.273	−3.540	1.00	31.85	A	C
ATOM	45	CG	GLU	A	818	7.228	64.650	−4.033	1.00	35.45	A	C
ATOM	46	CD	GLU	A	818	6.011	65.460	−4.446	1.00	36.12	A	C
ATOM	47	OE1	GLU	A	818	6.193	66.667	−4.710	1.00	36.77	A	O
ATOM	48	OE2	GLU	A	818	4.889	64.894	−4.510	1.00	34.70	A	O
ATOM	49	C	GLU	A	818	8.884	62.774	−2.097	1.00	30.93	A	C
ATOM	50	O	GLU	A	818	8.411	62.680	−0.958	1.00	30.09	A	O
ATOM	51	N	GLU	A	819	10.120	63.213	−2.342	1.00	30.52	A	N
ATOM	52	CA	GLU	A	819	11.017	63.635	−1.265	1.00	31.39	A	C
ATOM	53	CB	GLU	A	819	12.291	64.276	−1.836	1.00	29.12	A	C
ATOM	54	CG	GLU	A	819	13.384	63.303	−2.288	1.00	28.07	A	C
ATOM	55	CD	GLU	A	819	13.967	62.480	−1.138	1.00	26.19	A	C
ATOM	56	OE1	GLU	A	819	13.771	62.869	0.031	1.00	27.05	A	O
ATOM	57	OE2	GLU	A	819	14.632	61.455	−1.402	1.00	23.85	A	O
ATOM	58	C	GLU	A	819	10.349	64.607	−0.297	1.00	33.23	A	C
ATOM	59	O	GLU	A	819	10.489	64.477	0.923	1.00	34.49	A	O
ATOM	60	N	ARG	A	820	9.616	65.571	−0.843	1.00	34.22	A	N
ATOM	61	CA	ARG	A	820	8.917	66.574	−0.042	1.00	35.27	A	C
ATOM	62	CB	ARG	A	820	8.063	67.444	−0.973	1.00	36.97	A	C
ATOM	63	CG	ARG	A	820	7.375	68.619	−0.321	1.00	41.68	A	C
ATOM	64	CD	ARG	A	820	5.891	68.350	−0.106	1.00	46.06	A	C
ATOM	65	NE	ARG	A	820	5.539	68.200	1.306	1.00	49.53	A	N
ATOM	66	CZ	ARG	A	820	5.588	69.176	2.213	1.00	51.16	A	C
ATOM	67	NH1	ARG	A	820	5.978	70.398	1.867	1.00	50.30	A	N
ATOM	68	NH2	ARG	A	820	5.242	68.926	3.471	1.00	51.02	A	N
ATOM	69	C	ARG	A	820	8.046	65.991	1.087	1.00	34.18	A	C
ATOM	70	O	ARG	A	820	7.749	66.681	2.060	1.00	35.87	A	O
ATOM	71	N	HIS	A	821	7.638	64.730	0.964	1.00	32.13	A	N
ATOM	72	CA	HIS	A	821	6.809	64.097	1.980	1.00	29.99	A	C
ATOM	73	CB	HIS	A	821	5.700	63.251	1.327	1.00	31.61	A	C
ATOM	74	CG	HIS	A	821	4.699	64.054	0.547	1.00	35.95	A	C
ATOM	75	CD2	HIS	A	821	4.203	63.889	−0.703	1.00	35.71	A	C
ATOM	76	ND1	HIS	A	821	4.121	65.205	1.038	1.00	35.92	A	N
ATOM	77	CE1	HIS	A	821	3.319	65.719	0.122	1.00	35.31	A	C
ATOM	78	NE2	HIS	A	821	3.351	64.940	−0.943	1.00	34.98	A	N
ATOM	79	C	HIS	A	821	7.630	63.228	2.937	1.00	30.47	A	C
ATOM	80	O	HIS	A	821	7.084	62.609	3.845	1.00	31.60	A	O
ATOM	81	N	LEU	A	822	8.938	63.155	2.746	1.00	29.14	A	N
ATOM	82	CA	LEU	A	822	9.734	62.357	3.669	1.00	30.38	A	C
ATOM	83	CB	LEU	A	822	10.779	61.516	2.911	1.00	28.09	A	C
ATOM	84	CG	LEU	A	822	10.229	60.403	1.992	1.00	27.43	A	C
ATOM	85	CD1	LEU	A	822	11.359	59.787	1.205	1.00	25.73	A	C
ATOM	86	CD2	LEU	A	822	9.504	59.322	2.811	1.00	24.78	A	C
ATOM	87	C	LEU	A	822	10.402	63.296	4.678	1.00	30.74	A	C
ATOM	88	O	LEU	A	822	11.342	64.017	4.353	1.00	31.28	A	O
ATOM	89	N	LYS	A	823	9.893	63.305	5.903	1.00	31.44	A	N
ATOM	90	CA	LYS	A	823	10.455	64.169	6.934	1.00	31.93	A	C
ATOM	91	CB	LYS	A	823	9.367	64.596	7.917	1.00	32.76	A	C
ATOM	92	CG	LYS	A	823	8.439	65.660	7.385	1.00	35.51	A	C
ATOM	93	CD	LYS	A	823	7.557	65.135	6.284	1.00	37.19	A	C
ATOM	94	CE	LYS	A	823	6.627	66.226	5.808	1.00	36.96	A	C
ATOM	95	NZ	LYS	A	823	7.411	67.355	5.255	1.00	39.29	A	N
ATOM	96	C	LYS	A	823	11.601	63.513	7.700	1.00	30.88	A	C
ATOM	97	O	LYS	A	823	11.407	62.522	8.405	1.00	29.92	A	O
ATOM	98	N	TYR	A	824	12.793	64.080	7.549	1.00	30.36	A	N
ATOM	99	CA	TYR	A	824	13.986	63.584	8.225	1.00	31.67	A	C
ATOM	100	CB	TYR	A	824	15.169	64.521	7.956	1.00	31.69	A	C
ATOM	101	CG	TYR	A	824	16.378	64.226	8.821	1.00	33.19	A	C
ATOM	102	CD1	TYR	A	824	17.277	63.221	8.476	1.00	34.10	A	C
ATOM	103	CE1	TYR	A	824	18.358	62.910	9.281	1.00	34.40	A	C
ATOM	104	CD2	TYR	A	824	16.598	64.921	10.006	1.00	34.17	A	C
ATOM	105	CE2	TYR	A	824	17.681	64.613	10.822	1.00	36.17	A	C

TABLE 2-continued

ATOM	106	CZ	TYR	A	824	18.555	63.603	10.452	1.00	36.25	A	C
ATOM	107	OH	TYR	A	824	19.612	63.258	11.263	1.00	37.45	A	O
ATOM	108	C	TYR	A	824	13.788	63.481	9.738	1.00	32.15	A	C
ATOM	109	O	TYR	A	824	13.279	64.406	10.369	1.00	29.97	A	O
ATOM	110	N	ILE	A	825	14.190	62.356	10.321	1.00	33.67	A	N
ATOM	111	CA	ILE	A	825	14.065	62.188	11.762	1.00	34.78	A	C
ATOM	112	CB	ILE	A	825	13.177	60.959	12.123	1.00	34.51	A	C
ATOM	113	CG2	ILE	A	825	13.321	60.619	13.600	1.00	32.74	A	C
ATOM	114	CG1	ILE	A	825	11.703	61.262	11.801	1.00	33.78	A	C
ATOM	115	CD1	ILE	A	825	10.735	60.128	12.156	1.00	31.83	A	C
ATOM	116	C	ILE	A	825	15.458	62.040	12.380	1.00	36.16	A	C
ATOM	117	O	ILE	A	825	15.781	62.696	13.377	1.00	36.26	A	O
ATOM	118	N	SER	A	826	16.284	61.194	11.770	1.00	36.00	A	N
ATOM	119	CA	SER	A	826	17.645	60.963	12.247	1.00	37.27	A	C
ATOM	120	CB	SER	A	826	17.637	60.362	13.653	1.00	37.84	A	C
ATOM	121	OG	SER	A	826	17.216	59.011	13.615	1.00	41.26	A	O
ATOM	122	C	SER	A	826	18.383	60.017	11.312	1.00	36.08	A	C
ATOM	123	O	SER	A	826	17.785	59.401	10.433	1.00	36.11	A	O
ATOM	124	N	GLN	A	827	19.693	59.914	11.499	1.00	35.73	A	N
ATOM	125	CA	GLN	A	827	20.495	59.034	10.672	1.00	35.07	A	C
ATOM	126	CB	GLN	A	827	21.853	59.660	10.372	1.00	36.39	A	C
ATOM	127	CG	GLN	A	827	21.839	60.555	9.144	1.00	41.54	A	C
ATOM	128	CD	GLN	A	827	23.123	61.333	8.970	1.00	44.27	A	C
ATOM	129	OE1	GLN	A	827	23.527	62.094	9.852	1.00	46.01	A	O
ATOM	130	NE2	GLN	A	827	23.773	61.147	7.830	1.00	46.06	A	N
ATOM	131	C	GLN	A	827	20.685	57.706	11.362	1.00	34.12	A	C
ATOM	132	O	GLN	A	827	20.851	57.646	12.579	1.00	32.64	A	O
ATOM	133	N	LEU	A	828	20.644	56.639	10.568	1.00	32.89	A	N
ATOM	134	CA	LEU	A	828	20.818	55.294	11.084	1.00	30.70	A	C
ATOM	135	CB	LEU	A	828	19.852	54.338	10.380	1.00	29.69	A	C
ATOM	136	CG	LEU	A	828	18.371	54.593	10.675	1.00	30.57	A	C
ATOM	137	CD1	LEU	A	828	17.500	53.653	9.851	1.00	28.22	A	C
ATOM	138	CD2	LEU	A	828	18.107	54.400	12.174	1.00	27.72	A	C
ATOM	139	C	LEU	A	828	22.253	54.793	10.937	1.00	28.35	A	C
ATOM	140	O	LEU	A	828	22.695	53.966	11.716	1.00	27.97	A	O
ATOM	141	N	GLY	A	829	22.981	55.293	9.945	1.00	29.46	A	N
ATOM	142	CA	GLY	A	829	24.354	54.853	9.756	1.00	28.42	A	C
ATOM	143	C	GLY	A	829	24.780	54.760	8.302	1.00	27.74	A	C
ATOM	144	O	GLY	A	829	23.968	54.944	7.394	1.00	25.98	A	O
ATOM	145	N	LYS	A	830	26.064	54.472	8.092	1.00	27.82	A	N
ATOM	146	CA	LYS	A	830	26.658	54.339	6.765	1.00	28.70	A	C
ATOM	147	CB	LYS	A	830	27.716	55.418	6.542	1.00	31.68	A	C
ATOM	148	CG	LYS	A	830	28.729	55.005	5.483	1.00	38.00	A	C
ATOM	149	CD	LYS	A	830	30.008	55.815	5.517	1.00	42.10	A	C
ATOM	150	CE	LYS	A	830	31.047	55.190	4.587	1.00	44.14	A	C
ATOM	151	NZ	LYS	A	830	32.187	56.113	4.301	1.00	46.55	A	N
ATOM	152	C	LYS	A	830	27.327	52.968	6.636	1.00	27.26	A	C
ATOM	153	O	LYS	A	830	28.028	52.535	7.546	1.00	27.49	A	O
ATOM	154	N	GLY	A	831	27.131	52.300	5.501	1.00	25.76	A	N
ATOM	155	CA	GLY	A	831	27.716	50.985	5.302	1.00	24.03	A	C
ATOM	156	C	GLY	A	831	28.751	50.940	4.196	1.00	23.33	A	C
ATOM	157	O	GLY	A	831	29.557	51.861	4.063	1.00	23.56	A	O
ATOM	158	N	ASN	A	832	28.704	49.869	3.401	1.00	23.05	A	N
ATOM	159	CA	ASN	A	832	29.613	49.614	2.278	1.00	21.30	A	C
ATOM	160	CB	ASN	A	832	29.756	48.104	2.063	1.00	19.33	A	C
ATOM	161	CG	ASN	A	832	30.556	47.424	3.150	1.00	18.24	A	C
ATOM	162	OD1	ASN	A	832	31.731	47.712	3.315	1.00	18.72	A	O
ATOM	163	ND2	ASN	A	832	29.927	46.511	3.890	1.00	13.29	A	N
ATOM	164	C	ASN	A	832	29.182	50.222	0.946	1.00	22.90	A	C
ATOM	165	O	ASN	A	832	29.986	50.315	0.018	1.00	22.04	A	O
ATOM	166	N	PHE	A	833	27.913	50.604	0.829	1.00	24.50	A	N
ATOM	167	CA	PHE	A	833	27.439	51.157	−0.434	1.00	25.47	A	C
ATOM	168	CB	PHE	A	833	26.633	50.109	−1.197	1.00	24.25	A	C
ATOM	169	CG	PHE	A	833	27.366	48.819	−1.401	1.00	24.66	A	C
ATOM	170	CD1	PHE	A	833	27.226	47.778	−0.497	1.00	24.28	A	C
ATOM	171	CD2	PHE	A	833	28.215	48.650	−2.485	1.00	23.57	A	C
ATOM	172	CE1	PHE	A	833	27.919	46.591	−0.672	1.00	23.07	A	C
ATOM	173	CE2	PHE	A	833	28.910	47.464	−2.662	1.00	23.02	A	C
ATOM	174	CZ	PHE	A	833	28.761	46.437	−1.755	1.00	21.21	A	C
ATOM	175	C	PHE	A	833	26.618	52.426	−0.333	1.00	26.66	A	C
ATOM	176	O	PHE	A	833	26.543	53.175	−1.299	1.00	29.44	A	O
ATOM	177	N	GLY	A	834	26.002	52.667	0.822	1.00	26.24	A	N
ATOM	178	CA	GLY	A	834	25.199	53.859	0.986	1.00	26.25	A	C
ATOM	179	C	GLY	A	834	24.949	54.274	2.428	1.00	29.49	A	C
ATOM	180	O	GLY	A	834	25.604	53.809	3.370	1.00	30.21	A	O
ATOM	181	N	SER	A	835	23.990	55.171	2.610	1.00	29.04	A	N
ATOM	182	CA	SER	A	835	23.665	55.644	3.938	1.00	30.18	A	C
ATOM	183	CB	SER	A	835	24.092	57.104	4.099	1.00	29.43	A	C
ATOM	184	OG	SER	A	835	24.164	57.744	2.840	1.00	32.95	A	O
ATOM	185	C	SER	A	835	22.178	55.480	4.138	1.00	29.88	A	C

TABLE 2-continued

ATOM	186	O	SER	A	835	21.420	55.418	3.166	1.00	31.77	A	O
ATOM	187	N	VAL	A	836	21.770	55.404	5.400	1.00	28.84	A	N
ATOM	188	CA	VAL	A	836	20.373	55.201	5.752	1.00	27.14	A	C
ATOM	189	CB	VAL	A	836	20.167	53.788	6.323	1.00	26.52	A	C
ATOM	190	CG1	VAL	A	836	18.684	53.558	6.635	1.00	26.80	A	C
ATOM	191	CG2	VAL	A	836	20.697	52.747	5.336	1.00	26.73	A	C
ATOM	192	C	VAL	A	836	19.874	56.195	6.783	1.00	28.59	A	C
ATOM	193	O	VAL	A	836	20.559	56.489	7.771	1.00	27.84	A	O
ATOM	194	N	GLU	A	837	18.666	56.698	6.550	1.00	28.68	A	N
ATOM	195	CA	GLU	A	837	18.032	57.646	7.460	1.00	29.30	A	C
ATOM	196	CB	GLU	A	837	17.847	58.998	6.780	1.00	29.51	A	C
ATOM	197	CG	GLU	A	837	19.100	59.647	6.279	1.00	29.26	A	C
ATOM	198	CD	GLU	A	837	18.836	61.075	5.896	1.00	28.21	A	C
ATOM	199	OE1	GLU	A	837	17.661	61.375	5.602	1.00	29.43	A	O
ATOM	200	OE2	GLU	A	837	19.781	61.890	5.880	1.00	29.52	A	O
ATOM	201	C	GLU	A	837	16.656	57.143	7.902	1.00	30.42	A	C
ATOM	202	O	GLU	A	837	16.020	56.341	7.206	1.00	30.43	A	O
ATOM	203	N	LEU	A	838	16.201	57.618	9.061	1.00	30.98	A	N
ATOM	204	CA	LEU	A	838	14.886	57.253	9.584	1.00	30.21	A	C
ATOM	205	CB	LEU	A	838	14.921	57.034	11.100	1.00	30.08	A	C
ATOM	206	CG	LEU	A	838	13.571	56.846	11.822	1.00	30.36	A	C
ATOM	207	CD1	LEU	A	838	12.825	55.640	11.294	1.00	29.07	A	C
ATOM	208	CD2	LEU	A	838	13.812	56.679	13.297	1.00	29.13	A	C
ATOM	209	C	LEU	A	838	14.002	58.437	9.271	1.00	31.11	A	C
ATOM	210	O	LEU	A	838	14.210	59.528	9.804	1.00	33.21	A	O
ATOM	211	N	CYS	A	839	13.030	58.225	8.392	1.00	30.58	A	N
ATOM	212	CA	CYS	A	839	12.113	59.282	7.996	1.00	31.03	A	C
ATOM	213	CB	CYS	A	839	12.262	59.581	6.503	1.00	29.27	A	C
ATOM	214	SG	CYS	A	839	13.914	59.993	5.930	1.00	27.80	A	S
ATOM	215	C	CYS	A	839	10.654	58.916	8.261	1.00	32.73	A	C
ATOM	216	O	CYS	A	839	10.316	57.768	8.563	1.00	33.99	A	O
ATOM	217	N	ARG	A	840	9.780	59.900	8.134	1.00	32.93	A	N
ATOM	218	CA	ARG	A	840	8.372	59.642	8.312	1.00	34.97	A	C
ATOM	219	CB	ARG	A	840	7.820	60.439	9.499	1.00	37.08	A	C
ATOM	220	CG	ARG	A	840	6.325	60.238	9.734	1.00	39.75	A	C
ATOM	221	CD	ARG	A	840	5.744	61.214	10.764	1.00	42.91	A	C
ATOM	222	NE	ARG	A	840	6.009	60.817	12.145	1.00	45.02	A	N
ATOM	223	CZ	ARG	A	840	6.779	61.492	12.995	1.00	46.42	A	C
ATOM	224	NH1	ARG	A	840	7.378	62.617	12.616	1.00	45.99	A	N
ATOM	225	NH2	ARG	A	840	6.950	61.036	14.231	1.00	46.11	A	N
ATOM	226	C	ARG	A	840	7.685	60.072	7.029	1.00	34.39	A	C
ATOM	227	O	ARG	A	840	7.911	61.177	6.544	1.00	33.96	A	O
ATOM	228	N	TYR	A	841	6.885	59.184	6.452	1.00	36.23	A	N
ATOM	229	CA	TYR	A	841	6.145	59.516	5.241	1.00	38.35	A	C
ATOM	230	CB	TYR	A	841	5.696	58.246	4.511	1.00	38.71	A	C
ATOM	231	CG	TYR	A	841	4.982	58.516	3.206	1.00	38.68	A	C
ATOM	232	CD1	TYR	A	841	5.490	59.430	2.294	1.00	37.37	A	C
ATOM	233	CE1	TYR	A	841	4.859	59.673	1.101	1.00	36.58	A	C
ATOM	234	CD2	TYR	A	841	3.811	57.848	2.878	1.00	39.63	A	C
ATOM	235	CE2	TYR	A	841	3.172	58.085	1.680	1.00	39.84	A	C
ATOM	236	CZ	TYR	A	841	3.703	58.998	0.798	1.00	38.61	A	C
ATOM	237	OH	TYR	A	841	3.066	59.234	−0.397	1.00	41.90	A	O
ATOM	238	C	TYR	A	841	4.947	60.259	5.801	1.00	40.68	A	C
ATOM	239	O	TYR	A	841	4.146	59.679	6.531	1.00	40.74	A	O
ATOM	240	N	ASP	A	842	4.832	61.543	5.474	1.00	43.88	A	N
ATOM	241	CA	ASP	A	842	3.755	62.370	6.009	1.00	46.15	A	C
ATOM	242	CB	ASP	A	842	4.326	63.219	7.152	1.00	46.02	A	C
ATOM	243	CG	ASP	A	842	3.358	63.397	8.303	1.00	46.16	A	C
ATOM	244	OD1	ASP	A	842	2.749	62.395	8.730	1.00	46.36	A	O
ATOM	245	OD2	ASP	A	842	3.225	64.538	8.797	1.00	44.93	A	O
ATOM	246	C	ASP	A	842	3.135	63.277	4.950	1.00	48.03	A	C
ATOM	247	O	ASP	A	842	3.262	64.500	5.029	1.00	47.67	A	O
ATOM	248	N	PRO	A	843	2.453	62.688	3.948	1.00	50.40	A	N
ATOM	249	CD	PRO	A	843	2.212	61.242	3.809	1.00	50.93	A	C
ATOM	250	CA	PRO	A	843	1.801	63.427	2.858	1.00	51.87	A	C
ATOM	251	CB	PRO	A	843	0.980	62.348	2.154	1.00	51.29	A	C
ATOM	252	CG	PRO	A	843	1.792	61.125	2.359	1.00	50.63	A	C
ATOM	253	C	PRO	A	843	0.923	64.556	3.389	1.00	53.34	A	C
ATOM	254	O	PRO	A	843	0.848	65.633	2.798	1.00	54.36	A	O
ATOM	255	N	LEU	A	844	0.263	64.295	4.511	1.00	54.96	A	N
ATOM	256	CA	LEU	A	844	−0.612	65.273	5.144	1.00	56.98	A	C
ATOM	257	CB	LEU	A	844	−1.832	64.569	5.745	1.00	57.16	A	C
ATOM	258	CG	LEU	A	844	−2.540	63.518	4.878	1.00	57.83	A	C
ATOM	259	CD1	LEU	A	844	−2.826	64.080	3.490	1.00	57.39	A	C
ATOM	260	CD2	LEU	A	844	−1.667	62.287	4.770	1.00	58.93	A	C
ATOM	261	C	LEU	A	844	0.158	66.004	6.245	1.00	58.02	A	C
ATOM	262	O	LEU	A	844	1.173	65.510	6.736	1.00	58.53	A	O
ATOM	263	N	GLY	A	845	−0.320	67.178	6.636	1.00	59.34	A	N
ATOM	264	CA	GLY	A	845	0.366	67.926	7.676	1.00	60.48	A	C
ATOM	265	C	GLY	A	845	0.607	67.135	8.956	1.00	61.50	A	C

TABLE 2-continued

ATOM	266	O	GLY	A	845	1.748	66.986	9.400	1.00	61.55	A	O
ATOM	267	N	ASP	A	846	−0.471	66.631	9.551	1.00	61.30	A	N
ATOM	268	CA	ASP	A	846	−0.383	65.862	10.785	1.00	61.54	A	C
ATOM	269	CB	ASP	A	846	−1.731	65.199	11.100	1.00	63.49	A	C
ATOM	270	CG	ASP	A	846	−2.244	64.334	9.960	1.00	64.35	A	C
ATOM	271	OD1	ASP	A	846	−3.385	63.835	10.056	1.00	66.21	A	O
ATOM	272	OD2	ASP	A	846	−1.510	64.148	8.968	1.00	65.16	A	O
ATOM	273	C	ASP	A	846	0.700	64.806	10.684	1.00	61.10	A	C
ATOM	274	O	ASP	A	846	0.805	64.108	9.677	1.00	61.50	A	O
ATOM	275	N	ASN	A	847	1.501	64.690	11.735	1.00	59.87	A	N
ATOM	276	CA	ASN	A	847	2.589	63.723	11.763	1.00	57.70	A	C
ATOM	277	CB	ASN	A	847	3.512	64.038	12.924	1.00	58.23	A	C
ATOM	278	CG	ASN	A	847	4.087	65.416	12.826	1.00	58.62	A	C
ATOM	279	OD1	ASN	A	847	4.999	65.663	12.039	1.00	59.48	A	O
ATOM	280	ND2	ASN	A	847	3.543	66.337	13.607	1.00	59.51	A	N
ATOM	281	C	ASN	A	847	2.083	62.304	11.895	1.00	55.91	A	C
ATOM	282	O	ASN	A	847	2.803	61.426	12.374	1.00	56.51	A	O
ATOM	283	N	THR	A	848	0.845	62.085	11.465	1.00	53.41	A	N
ATOM	284	CA	THR	A	848	0.222	60.771	11.541	1.00	51.20	A	C
ATOM	285	CB	THR	A	848	−1.273	60.836	11.136	1.00	50.55	A	C
ATOM	286	OG1	THR	A	848	−1.390	61.250	9.768	1.00	49.25	A	O
ATOM	287	CG2	THR	A	848	−2.023	61.818	12.023	1.00	49.29	A	C
ATOM	288	C	THR	A	848	0.920	59.735	10.663	1.00	50.05	A	C
ATOM	289	O	THR	A	848	0.606	58.547	10.732	1.00	51.27	A	O
ATOM	290	N	GLY	A	849	1.866	60.184	9.845	1.00	47.22	A	N
ATOM	291	CA	GLY	A	849	2.582	59.274	8.965	1.00	44.27	A	C
ATOM	292	C	GLY	A	849	3.322	58.124	9.632	1.00	41.86	A	C
ATOM	293	O	GLY	A	849	3.518	58.109	10.848	1.00	42.65	A	O
ATOM	294	N	ALA	A	850	3.750	57.159	8.822	1.00	40.05	A	N
ATOM	295	CA	ALA	A	850	4.467	55.984	9.315	1.00	37.02	A	C
ATOM	296	CB	ALA	A	850	3.994	54.730	8.571	1.00	36.14	A	C
ATOM	297	C	ALA	A	850	5.979	56.103	9.188	1.00	36.11	A	C
ATOM	298	O	ALA	A	850	6.501	56.891	8.397	1.00	35.06	A	O
ATOM	299	N	LEU	A	851	6.682	55.309	9.982	1.00	34.16	A	N
ATOM	300	CA	LEU	A	851	8.130	55.307	9.930	1.00	33.37	A	C
ATOM	301	CB	LEU	A	851	8.704	54.832	11.264	1.00	35.31	A	C
ATOM	302	CG	LEU	A	851	9.165	55.901	12.257	1.00	36.20	A	C
ATOM	303	CD1	LEU	A	851	8.253	57.120	12.182	1.00	36.82	A	C
ATOM	304	CD2	LEU	A	851	9.181	55.297	13.664	1.00	34.32	A	C
ATOM	305	C	LEU	A	851	8.611	54.394	8.806	1.00	31.96	A	C
ATOM	306	O	LEU	A	851	8.015	53.354	8.540	1.00	31.31	A	O
ATOM	307	N	VAL	A	852	9.682	54.802	8.134	1.00	31.01	A	N
ATOM	308	CA	VAL	A	852	10.258	54.012	7.055	1.00	27.90	A	C
ATOM	309	CB	VAL	A	852	9.715	54.441	5.672	1.00	26.77	A	C
ATOM	310	CG1	VAL	A	852	8.205	54.243	5.603	1.00	28.29	A	C
ATOM	311	CG2	VAL	A	852	10.065	55.876	5.416	1.00	24.56	A	C
ATOM	312	C	VAL	A	852	11.773	54.200	7.047	1.00	29.02	A	C
ATOM	313	O	VAL	A	852	12.286	55.216	7.528	1.00	28.76	A	O
ATOM	314	N	ALA	A	853	12.486	53.212	6.513	1.00	28.28	A	N
ATOM	315	CA	ALA	A	853	13.937	53.293	6.404	1.00	27.51	A	C
ATOM	316	CB	ALA	A	853	14.564	51.949	6.642	1.00	27.05	A	C
ATOM	317	C	ALA	A	853	14.218	53.749	4.985	1.00	28.18	A	C
ATOM	318	O	ALA	A	853	13.746	53.132	4.016	1.00	28.55	A	O
ATOM	319	N	VAL	A	854	14.983	54.828	4.857	1.00	26.18	A	N
ATOM	320	CA	VAL	A	854	15.297	55.366	3.546	1.00	25.26	A	C
ATOM	321	CB	VAL	A	854	14.806	56.815	3.404	1.00	24.58	A	C
ATOM	322	CG1	VAL	A	854	15.175	57.355	2.020	1.00	25.67	A	C
ATOM	323	CG2	VAL	A	854	13.306	56.868	3.640	1.00	20.74	A	C
ATOM	324	C	VAL	A	854	16.779	55.343	3.275	1.00	25.34	A	C
ATOM	325	O	VAL	A	854	17.523	56.142	3.827	1.00	27.35	A	O
ATOM	326	N	LYS	A	855	17.211	54.430	2.418	1.00	24.66	A	N
ATOM	327	CA	LYS	A	855	18.622	54.339	2.091	1.00	25.16	A	C
ATOM	328	CB	LYS	A	855	19.087	52.877	2.050	1.00	22.54	A	C
ATOM	329	CG	LYS	A	855	20.264	52.682	1.088	1.00	20.44	A	C
ATOM	330	CD	LYS	A	855	20.761	51.253	0.972	1.00	18.74	A	C
ATOM	331	CE	LYS	A	855	21.444	50.753	2.237	1.00	18.04	A	C
ATOM	332	NZ	LYS	A	855	22.347	49.633	1.878	1.00	16.00	A	N
ATOM	333	C	LYS	A	855	18.944	54.987	0.746	1.00	26.42	A	C
ATOM	334	O	LYS	A	855	18.185	54.861	−0.214	1.00	23.35	A	O
ATOM	335	N	GLN	A	856	20.071	55.693	0.702	1.00	27.46	A	N
ATOM	336	CA	GLN	A	856	20.557	56.315	−0.522	1.00	29.59	A	C
ATOM	337	CB	GLN	A	856	20.792	57.818	−0.325	1.00	29.19	A	C
ATOM	338	CG	GLN	A	856	21.044	58.568	−1.637	1.00	32.25	A	C
ATOM	339	CD	GLN	A	856	21.048	60.101	−1.489	1.00	33.60	A	C
ATOM	340	OE1	GLN	A	856	21.849	60.654	−0.742	1.00	38.48	A	O
ATOM	341	NE2	GLN	A	856	20.157	60.782	−2.213	1.00	28.07	A	N
ATOM	342	C	GLN	A	856	21.882	55.624	−0.875	1.00	30.88	A	C
ATOM	343	O	GLN	A	856	22.804	55.563	−0.054	1.00	31.97	A	O
ATOM	344	N	LEU	A	857	21.967	55.088	−2.085	1.00	32.50	A	N
ATOM	345	CA	LEU	A	857	23.178	54.412	−2.542	1.00	35.93	A	C

TABLE 2-continued

ATOM	346	CB	LEU	A	857	22.837	53.379	−3.620	1.00	33.15	A	C
ATOM	347	CG	LEU	A	857	21.875	52.268	−3.202	1.00	31.85	A	C
ATOM	348	CD1	LEU	A	857	21.562	51.361	−4.379	1.00	31.75	A	C
ATOM	349	CD2	LEU	A	857	22.494	51.484	−2.072	1.00	31.93	A	C
ATOM	350	C	LEU	A	857	24.202	55.386	−3.114	1.00	38.69	A	C
ATOM	351	O	LEU	A	857	23.845	56.347	−3.796	1.00	37.21	A	O
ATOM	352	N	GLN	A	858	25.473	55.146	−2.814	1.00	43.02	A	N
ATOM	353	CA	GLN	A	858	26.540	55.979	−3.347	1.00	48.51	A	C
ATOM	354	CB	GLN	A	858	27.899	55.516	−2.808	1.00	49.56	A	C
ATOM	355	CG	GLN	A	858	29.091	56.039	−3.601	1.00	52.69	A	C
ATOM	356	CD	GLN	A	858	30.384	55.277	−3.320	1.00	55.55	A	C
ATOM	357	OE1	GLN	A	858	30.403	54.044	−3.301	1.00	56.97	A	O
ATOM	358	NE2	GLN	A	858	31.474	56.013	−3.113	1.00	56.46	A	N
ATOM	359	C	GLN	A	858	26.465	55.749	−4.854	1.00	51.62	A	C
ATOM	360	O	GLN	A	858	26.836	54.687	−5.354	1.00	52.30	A	O
ATOM	361	N	HIS	A	859	25.968	56.737	−5.579	1.00	56.16	A	N
ATOM	362	CA	HIS	A	859	25.827	56.591	−7.019	1.00	59.85	A	C
ATOM	363	CB	HIS	A	859	24.361	56.781	−7.414	1.00	60.11	A	C
ATOM	364	CG	HIS	A	859	24.025	56.251	−8.772	1.00	61.57	A	C
ATOM	365	CD2	HIS	A	859	23.561	56.872	−9.882	1.00	62.54	A	C
ATOM	366	ND1	HIS	A	859	24.157	54.921	−9.103	1.00	62.61	A	N
ATOM	367	CE1	HIS	A	859	23.789	54.743	−10.360	1.00	63.08	A	C
ATOM	368	NE2	HIS	A	859	23.423	55.911	−10.855	1.00	63.34	A	N
ATOM	369	C	HIS	A	859	26.699	57.605	−7.744	1.00	61.51	A	C
ATOM	370	O	HIS	A	859	26.380	58.794	−7.795	1.00	62.00	A	O
ATOM	371	N	SER	A	860	27.811	57.129	−8.291	1.00	63.34	A	N
ATOM	372	CA	SER	A	860	28.726	57.996	−9.018	1.00	64.52	A	C
ATOM	373	CB	SER	A	860	30.132	57.916	−8.416	1.00	65.20	A	C
ATOM	374	OG	SER	A	860	30.108	58.201	−7.025	1.00	65.35	A	O
ATOM	375	C	SER	A	860	28.746	57.574	−10.480	1.00	65.06	A	C
ATOM	376	O	SER	A	860	29.523	56.708	−10.886	1.00	64.96	A	O
ATOM	377	N	GLY	A	861	27.862	58.198	−11.252	1.00	65.21	A	N
ATOM	378	CA	GLY	A	861	27.738	57.924	−12.670	1.00	65.25	A	C
ATOM	379	C	GLY	A	861	26.374	58.427	−13.094	1.00	65.25	A	C
ATOM	380	O	GLY	A	861	25.606	58.885	−12.245	1.00	65.70	A	O
ATOM	381	N	PRO	A	862	26.032	58.368	−14.389	1.00	64.70	A	N
ATOM	382	CD	PRO	A	862	26.713	57.725	−15.526	1.00	65.03	A	C
ATOM	383	CA	PRO	A	862	24.707	58.854	−14.783	1.00	63.21	A	C
ATOM	384	CB	PRO	A	862	24.678	58.591	−16.287	1.00	63.52	A	C
ATOM	385	CG	PRO	A	862	25.548	57.375	−16.425	1.00	64.47	A	C
ATOM	386	C	PRO	A	862	23.598	58.107	−14.046	1.00	61.61	A	C
ATOM	387	O	PRO	A	862	23.425	56.904	−14.232	1.00	61.26	A	O
ATOM	388	N	ASP	A	863	22.865	58.823	−13.197	1.00	59.69	A	N
ATOM	389	CA	ASP	A	863	21.763	58.228	−12.444	1.00	56.82	A	C
ATOM	390	CB	ASP	A	863	20.950	59.303	−11.721	1.00	58.54	A	C
ATOM	391	CG	ASP	A	863	20.091	60.133	−12.680	1.00	59.27	A	C
ATOM	392	OD1	ASP	A	863	20.662	60.803	−13.574	1.00	60.57	A	O
ATOM	393	OD2	ASP	A	863	18.849	60.115	−12.541	1.00	58.02	A	O
ATOM	394	C	ASP	A	863	20.859	57.574	−13.461	1.00	54.16	A	C
ATOM	395	O	ASP	A	863	20.821	58.004	−14.612	1.00	54.94	A	O
ATOM	396	N	GLN	A	864	20.126	56.548	−13.044	1.00	49.49	A	N
ATOM	397	CA	GLN	A	864	19.212	55.875	−13.953	1.00	44.06	A	C
ATOM	398	CB	GLN	A	864	19.861	54.620	−14.509	1.00	46.96	A	C
ATOM	399	CG	GLN	A	864	21.098	54.950	−15.309	1.00	49.97	A	C
ATOM	400	CD	GLN	A	864	20.834	56.024	−16.348	1.00	51.95	A	C
ATOM	401	OE1	GLN	A	864	21.748	56.732	−16.769	1.00	54.75	A	O
ATOM	402	NE2	GLN	A	864	19.580	56.149	−16.769	1.00	53.04	A	N
ATOM	403	C	GLN	A	864	17.883	55.553	−13.297	1.00	39.54	A	C
ATOM	404	O	GLN	A	864	17.674	54.464	−12.767	1.00	37.98	A	O
ATOM	405	N	GLN	A	865	16.995	56.540	−13.343	1.00	34.60	A	N
ATOM	406	CA	GLN	A	865	15.671	56.455	−12.766	1.00	30.90	A	C
ATOM	407	CB	GLN	A	865	14.875	57.702	−13.173	1.00	29.99	A	C
ATOM	408	CG	GLN	A	865	13.395	57.657	−12.845	1.00	27.24	A	C
ATOM	409	CD	GLN	A	865	12.635	56.758	−13.792	1.00	25.91	A	C
ATOM	410	OE1	GLN	A	865	12.783	56.867	−15.013	1.00	26.96	A	O
ATOM	411	NE2	GLN	A	865	11.815	55.866	−13.241	1.00	26.05	A	N
ATOM	412	C	GLN	A	865	14.937	55.178	−13.164	1.00	30.14	A	C
ATOM	413	O	GLN	A	865	14.330	54.514	−12.317	1.00	29.46	A	O
ATOM	414	N	ARG	A	866	14.992	54.835	−14.446	1.00	28.26	A	N
ATOM	415	CA	ARG	A	866	14.339	53.630	−14.939	1.00	27.87	A	C
ATOM	416	CB	ARG	A	866	14.556	53.480	−16.442	1.00	30.08	A	C
ATOM	417	CG	ARG	A	866	13.762	54.460	−17.277	1.00	31.40	A	C
ATOM	418	CD	ARG	A	866	14.135	54.349	−18.744	1.00	30.86	A	C
ATOM	419	NE	ARG	A	866	13.327	55.237	−19.577	1.00	31.25	A	N
ATOM	420	CZ	ARG	A	866	13.453	56.561	−19.620	1.00	31.81	A	C
ATOM	421	NH1	ARG	A	866	12.661	57.268	−20.410	1.00	30.66	A	N
ATOM	422	NH2	ARG	A	866	14.370	57.181	−18.883	1.00	30.91	A	N
ATOM	423	C	ARG	A	866	14.843	52.386	−14.225	1.00	27.32	A	C
ATOM	424	O	ARG	A	866	14.039	51.559	−13.790	1.00	24.87	A	O
ATOM	425	N	ASP	A	867	16.165	52.247	−14.111	1.00	29.27	A	N

TABLE 2-continued

ATOM	426	CA	ASP	A	867	16.762	51.096	−13.420	1.00	30.55	A	C
ATOM	427	CB	ASP	A	867	18.287	51.202	−13.357	1.00	31.56	A	C
ATOM	428	CG	ASP	A	867	18.961	50.950	−14.701	1.00	34.40	A	C
ATOM	429	OD1	ASP	A	867	18.384	50.263	−15.578	1.00	35.17	A	O
ATOM	430	OD2	ASP	A	867	20.094	51.439	−14.869	1.00	36.88	A	O
ATOM	431	C	ASP	A	867	16.228	50.944	−12.001	1.00	31.08	A	C
ATOM	432	O	ASP	A	867	15.568	49.948	−11.694	1.00	31.13	A	O
ATOM	433	N	PHE	A	868	16.508	51.919	−11.134	1.00	31.00	A	N
ATOM	434	CA	PHE	A	868	16.018	51.844	−9.755	1.00	31.24	A	C
ATOM	435	CB	PHE	A	868	16.192	53.180	−9.024	1.00	30.81	A	C
ATOM	436	CG	PHE	A	868	17.597	53.467	−8.598	1.00	28.20	A	C
ATOM	437	CD1	PHE	A	868	18.591	53.669	−9.536	1.00	27.55	A	C
ATOM	438	CD2	PHE	A	868	17.921	53.533	−7.254	1.00	28.80	A	C
ATOM	439	CE1	PHE	A	868	19.884	53.931	−9.143	1.00	28.47	A	C
ATOM	440	CE2	PHE	A	868	19.207	53.793	−6.848	1.00	27.69	A	C
ATOM	441	CZ	PHE	A	868	20.194	53.993	−7.792	1.00	29.38	A	C
ATOM	442	C	PHE	A	868	14.536	51.487	−9.758	1.00	31.43	A	C
ATOM	443	O	PHE	A	868	14.076	50.687	−8.950	1.00	32.47	A	O
ATOM	444	N	GLN	A	869	13.800	52.095	−10.676	1.00	31.87	A	N
ATOM	445	CA	GLN	A	869	12.364	51.871	−10.814	1.00	33.84	A	C
ATOM	446	CB	GLN	A	869	11.827	52.814	−11.901	1.00	34.67	A	C
ATOM	447	CG	GLN	A	869	10.323	52.847	−12.055	1.00	39.76	A	C
ATOM	448	CD	GLN	A	869	9.621	53.521	−10.902	1.00	42.28	A	C
ATOM	449	OE1	GLN	A	869	8.422	53.775	−10.960	1.00	43.86	A	O
ATOM	450	NE2	GLN	A	869	10.366	53.815	−9.842	1.00	45.51	A	N
ATOM	451	C	GLN	A	869	12.053	50.405	−11.169	1.00	32.83	A	C
ATOM	452	O	GLN	A	869	11.157	49.777	−10.593	1.00	30.45	A	O
ATOM	453	N	ARG	A	870	12.807	49.868	−12.121	1.00	31.56	A	N
ATOM	454	CA	ARG	A	870	12.619	48.490	−12.567	1.00	29.61	A	C
ATOM	455	CB	ARG	A	870	13.578	48.192	−13.720	1.00	29.76	A	C
ATOM	456	CG	ARG	A	870	13.476	46.795	−14.306	1.00	30.49	A	C
ATOM	457	CD	ARG	A	870	14.608	46.577	−15.294	1.00	27.79	A	C
ATOM	458	NE	ARG	A	870	15.918	46.749	−14.671	1.00	26.84	A	N
ATOM	459	CZ	ARG	A	870	16.841	47.605	−15.098	1.00	27.83	A	C
ATOM	460	NH1	ARG	A	870	16.588	48.373	−16.152	1.00	24.51	A	N
ATOM	461	NH2	ARG	A	870	18.023	47.679	−14.485	1.00	25.65	A	N
ATOM	462	C	ARG	A	870	12.849	47.495	−11.438	1.00	29.71	A	C
ATOM	463	O	ARG	A	870	12.092	46.535	−11.266	1.00	30.22	A	O
ATOM	464	N	GLU	A	871	13.893	47.736	−10.658	1.00	30.06	A	N
ATOM	465	CA	GLU	A	871	14.244	46.851	−9.564	1.00	29.79	A	C
ATOM	466	CB	GLU	A	871	15.625	47.219	−9.054	1.00	29.83	A	C
ATOM	467	CG	GLU	A	871	16.677	47.061	−10.127	1.00	30.10	A	C
ATOM	468	CD	GLU	A	871	16.663	45.668	−10.734	1.00	32.26	A	C
ATOM	469	OE1	GLU	A	871	16.906	45.543	−11.956	1.00	33.53	A	O
ATOM	470	OE2	GLU	A	871	16.417	44.699	−9.985	1.00	32.71	A	O
ATOM	471	C	GLU	A	871	13.230	46.858	−8.435	1.00	32.02	A	C
ATOM	472	O	GLU	A	871	12.617	45.829	−8.127	1.00	31.99	A	O
ATOM	473	N	ILE	A	872	13.035	48.016	−7.822	1.00	33.05	A	N
ATOM	474	CA	ILE	A	872	12.081	48.115	−6.727	1.00	33.73	A	C
ATOM	475	CB	ILE	A	872	11.839	49.581	−6.320	1.00	34.18	A	C
ATOM	476	CG2	ILE	A	872	10.647	49.683	−5.409	1.00	34.71	A	C
ATOM	477	CG1	ILE	A	872	13.055	50.096	−5.563	1.00	35.67	A	C
ATOM	478	CD1	ILE	A	872	13.377	49.261	−4.352	1.00	33.28	A	C
ATOM	479	C	ILE	A	872	10.753	47.453	−7.061	1.00	32.84	A	C
ATOM	480	O	ILE	A	872	10.156	46.805	−6.200	1.00	33.81	A	O
ATOM	481	N	GLN	A	873	10.286	47.594	−8.301	1.00	31.38	A	N
ATOM	482	CA	GLN	A	873	9.014	46.972	−8.669	1.00	31.13	A	C
ATOM	483	CB	GLN	A	873	8.554	47.407	−10.060	1.00	31.19	A	C
ATOM	484	CG	GLN	A	873	8.194	48.867	−10.119	1.00	33.73	A	C
ATOM	485	CD	GLN	A	873	7.213	49.198	−11.218	1.00	36.91	A	C
ATOM	486	OE1	GLN	A	873	6.858	50.366	−11.396	1.00	41.17	A	O
ATOM	487	NE2	GLN	A	873	6.761	48.181	−11.960	1.00	35.88	A	N
ATOM	488	C	GLN	A	873	9.128	45.462	−8.614	1.00	30.57	A	C
ATOM	489	O	GLN	A	873	8.187	44.773	−8.209	1.00	30.27	A	O
ATOM	490	N	ILE	A	874	10.291	44.961	−9.022	1.00	28.38	A	N
ATOM	491	CA	ILE	A	874	10.571	43.538	−9.000	1.00	26.50	A	C
ATOM	492	CB	ILE	A	874	11.906	43.224	−9.738	1.00	25.96	A	C
ATOM	493	CG2	ILE	A	874	12.444	41.878	−9.304	1.00	25.39	A	C
ATOM	494	CG1	ILE	A	874	11.693	43.227	−11.252	1.00	23.07	A	C
ATOM	495	CD1	ILE	A	874	12.985	43.153	−12.033	1.00	24.11	A	C
ATOM	496	C	ILE	A	874	10.693	43.093	−7.542	1.00	27.93	A	C
ATOM	497	O	ILE	A	874	10.192	42.031	−7.157	1.00	27.66	A	O
ATOM	498	N	LEU	A	875	11.361	43.922	−6.737	1.00	27.30	A	N
ATOM	499	CA	LEU	A	875	11.576	43.629	−5.323	1.00	26.34	A	C
ATOM	500	CB	LEU	A	875	12.698	44.514	−4.769	1.00	25.39	A	C
ATOM	501	CG	LEU	A	875	14.108	44.249	−5.324	1.00	23.64	A	C
ATOM	502	CD1	LEU	A	875	15.052	45.341	−4.844	1.00	23.64	A	C
ATOM	503	CD2	LEU	A	875	14.610	42.897	−4.876	1.00	22.26	A	C
ATOM	504	C	LEU	A	875	10.308	43.802	−4.491	1.00	26.93	A	C
ATOM	505	O	LEU	A	875	10.068	43.056	−3.541	1.00	27.40	A	O

TABLE 2-continued

ATOM	506	N	LYS	A	876	9.486	44.774	−4.862	1.00	26.36	A	N
ATOM	507	CA	LYS	A	876	8.256	45.025	−4.134	1.00	27.17	A	C
ATOM	508	CB	LYS	A	876	7.669	46.380	−4.540	1.00	24.25	A	C
ATOM	509	CG	LYS	A	876	6.551	46.819	−3.634	1.00	24.74	A	C
ATOM	510	CD	LYS	A	876	5.952	48.150	−4.014	1.00	25.31	A	C
ATOM	511	CE	LYS	A	876	4.882	48.496	−3.008	1.00	24.35	A	C
ATOM	512	NZ	LYS	A	876	4.120	49.691	−3.413	1.00	28.04	A	N
ATOM	513	C	LYS	A	876	7.227	43.917	−4.369	1.00	29.28	A	C
ATOM	514	O	LYS	A	876	6.211	43.830	−3.666	1.00	32.41	A	O
ATOM	515	N	ALA	A	877	7.475	43.067	−5.358	1.00	28.69	A	N
ATOM	516	CA	ALA	A	877	6.533	41.990	−5.629	1.00	29.42	A	C
ATOM	517	CB	ALA	A	877	6.501	41.678	−7.130	1.00	27.23	A	C
ATOM	518	C	ALA	A	877	6.883	40.736	−4.814	1.00	29.56	A	C
ATOM	519	O	ALA	A	877	6.053	39.841	−4.653	1.00	28.54	A	O
ATOM	520	N	LEU	A	878	8.107	40.694	−4.288	1.00	29.51	A	N
ATOM	521	CA	LEU	A	878	8.585	39.573	−3.473	1.00	27.97	A	C
ATOM	522	CB	LEU	A	878	10.094	39.691	−3.250	1.00	26.08	A	C
ATOM	523	CG	LEU	A	878	10.959	39.783	−4.503	1.00	27.63	A	C
ATOM	524	CD1	LEU	A	878	12.350	40.250	−4.135	1.00	27.67	A	C
ATOM	525	CD2	LEU	A	878	10.991	38.444	−5.209	1.00	26.13	A	C
ATOM	526	C	LEU	A	878	7.896	39.556	−2.117	1.00	27.99	A	C
ATOM	527	O	LEU	A	878	7.899	40.560	−1.414	1.00	29.76	A	O
ATOM	528	N	HIS	A	879	7.308	38.425	−1.745	1.00	29.32	A	N
ATOM	529	CA	HIS	A	879	6.643	38.314	−0.451	1.00	31.36	A	C
ATOM	530	CB	HIS	A	879	5.130	38.240	−0.630	1.00	32.39	A	C
ATOM	531	CG	HIS	A	879	4.550	39.450	−1.285	1.00	39.51	A	C
ATOM	532	CD2	HIS	A	879	3.661	39.582	−2.296	1.00	40.92	A	C
ATOM	533	ND1	HIS	A	879	4.907	40.732	−0.918	1.00	42.50	A	N
ATOM	534	CE1	HIS	A	879	4.266	41.599	−1.679	1.00	43.10	A	C
ATOM	535	NE2	HIS	A	879	3.504	40.929	−2.525	1.00	44.26	A	N
ATOM	536	C	HIS	A	879	7.103	37.131	0.408	1.00	31.51	A	C
ATOM	537	O	HIS	A	879	6.948	35.968	0.022	1.00	31.05	A	O
ATOM	538	N	SER	A	880	7.666	37.454	1.575	1.00	30.02	A	N
ATOM	539	CA	SER	A	880	8.132	36.464	2.541	1.00	28.69	A	C
ATOM	540	CB	SER	A	880	9.564	36.052	2.251	1.00	27.94	A	C
ATOM	541	OG	SER	A	880	10.046	35.269	3.324	1.00	25.72	A	O
ATOM	542	C	SER	A	880	8.062	37.010	3.959	1.00	30.58	A	C
ATOM	543	O	SER	A	880	8.201	38.211	4.170	1.00	31.38	A	O
ATOM	544	N	ASP	A	881	7.848	36.132	4.933	1.00	31.77	A	N
ATOM	545	CA	ASP	A	881	7.762	36.568	6.322	1.00	32.73	A	C
ATOM	546	CB	ASP	A	881	7.001	35.543	7.169	1.00	36.42	A	C
ATOM	547	CG	ASP	A	881	5.539	35.439	6.786	1.00	41.67	A	C
ATOM	548	OD1	ASP	A	881	4.841	36.479	6.830	1.00	43.68	A	O
ATOM	549	OD2	ASP	A	881	5.090	34.318	6.446	1.00	43.38	A	O
ATOM	550	C	ASP	A	881	9.144	36.783	6.917	1.00	32.05	A	C
ATOM	551	O	ASP	A	881	9.284	37.257	8.046	1.00	31.81	A	O
ATOM	552	N	PHE	A	882	10.167	36.429	6.152	1.00	29.45	A	N
ATOM	553	CA	PHE	A	882	11.538	36.573	6.611	1.00	27.95	A	C
ATOM	554	CB	PHE	A	882	12.195	35.194	6.685	1.00	27.05	A	C
ATOM	555	CG	PHE	A	882	11.355	34.172	7.401	1.00	25.73	A	C
ATOM	556	CD1	PHE	A	882	11.060	34.318	8.741	1.00	24.96	A	C
ATOM	557	CD2	PHE	A	882	10.794	33.111	6.712	1.00	27.21	A	C
ATOM	558	CE1	PHE	A	882	10.209	33.427	9.388	1.00	26.21	A	C
ATOM	559	CE2	PHE	A	882	9.943	32.217	7.353	1.00	27.67	A	C
ATOM	560	CZ	PHE	A	882	9.650	32.378	8.691	1.00	24.82	A	C
ATOM	561	C	PHE	A	882	12.281	37.472	5.639	1.00	28.22	A	C
ATOM	562	O	PHE	A	882	13.422	37.210	5.282	1.00	27.42	A	O
ATOM	563	N	ILE	A	883	11.608	38.533	5.203	1.00	28.53	A	N
ATOM	564	CA	ILE	A	883	12.185	39.492	4.267	1.00	27.18	A	C
ATOM	565	CB	ILE	A	883	11.707	39.203	2.825	1.00	27.90	A	C
ATOM	566	CG2	ILE	A	883	11.013	40.427	2.239	1.00	27.92	A	C
ATOM	567	CG1	ILE	A	883	12.892	38.779	1.966	1.00	26.54	A	C
ATOM	568	CD1	ILE	A	883	13.414	37.448	2.314	1.00	23.32	A	C
ATOM	569	C	ILE	A	883	11.749	40.898	4.661	1.00	26.07	A	C
ATOM	570	O	ILE	A	883	10.608	41.101	5.070	1.00	26.87	A	O
ATOM	571	N	VAL	A	884	12.652	41.865	4.551	1.00	25.78	A	N
ATOM	572	CA	VAL	A	884	12.327	43.245	4.900	1.00	25.41	A	C
ATOM	573	CB	VAL	A	884	13.579	44.019	5.310	1.00	25.86	A	C
ATOM	574	CG1	VAL	A	884	13.209	45.438	5.667	1.00	25.61	A	C
ATOM	575	CG2	VAL	A	884	14.244	43.327	6.479	1.00	27.98	A	C
ATOM	576	C	VAL	A	884	11.677	43.928	3.701	1.00	25.52	A	C
ATOM	577	O	VAL	A	884	12.314	44.168	2.680	1.00	24.56	A	O
ATOM	578	N	LYS	A	885	10.398	44.246	3.851	1.00	26.64	A	N
ATOM	579	CA	LYS	A	885	9.605	44.855	2.798	1.00	26.33	A	C
ATOM	580	CB	LYS	A	885	8.174	45.059	3.301	1.00	27.25	A	C
ATOM	581	CG	LYS	A	885	7.258	43.868	3.055	1.00	29.12	A	C
ATOM	582	CD	LYS	A	885	5.912	44.038	3.735	1.00	31.39	A	C
ATOM	583	CE	LYS	A	885	6.068	44.055	5.241	1.00	31.87	A	C
ATOM	584	NZ	LYS	A	885	4.750	43.980	5.915	1.00	34.16	A	N
ATOM	585	C	LYS	A	885	10.100	46.150	2.162	1.00	26.24	A	C

TABLE 2-continued

ATOM	586	O	LYS	A	885	10.219	47.179	2.825	1.00	25.99	A	O
ATOM	587	N	TYR	A	886	10.409	46.081	0.870	1.00	25.58	A	N
ATOM	588	CA	TYR	A	886	10.808	47.264	0.125	1.00	24.39	A	C
ATOM	589	CB	TYR	A	886	11.464	46.875	−1.209	1.00	22.20	A	C
ATOM	590	CG	TYR	A	886	12.945	46.541	−1.126	1.00	21.86	A	C
ATOM	591	CD1	TYR	A	886	13.885	47.509	−0.768	1.00	20.74	A	C
ATOM	592	CE1	TYR	A	886	15.236	47.200	−0.681	1.00	19.63	A	C
ATOM	593	CD2	TYR	A	886	13.399	45.264	−1.397	1.00	20.05	A	C
ATOM	594	CE2	TYR	A	886	14.742	44.949	−1.313	1.00	19.69	A	C
ATOM	595	CZ	TYR	A	886	15.655	45.917	−0.953	1.00	20.05	A	C
ATOM	596	OH	TYR	A	886	16.992	45.596	−0.860	1.00	17.58	A	O
ATOM	597	C	TYR	A	886	9.461	47.948	−0.130	1.00	24.24	A	C
ATOM	598	O	TYR	A	886	8.430	47.273	−0.267	1.00	24.22	A	O
ATOM	599	N	ARG	A	887	9.452	49.272	−0.189	1.00	22.95	A	N
ATOM	600	CA	ARG	A	887	8.201	49.982	−0.406	1.00	23.16	A	C
ATOM	601	CB	ARG	A	887	7.854	50.811	0.828	1.00	23.19	A	C
ATOM	602	CG	ARG	A	887	7.348	49.964	1.972	1.00	27.32	A	C
ATOM	603	CD	ARG	A	887	6.714	50.824	3.034	1.00	31.16	A	C
ATOM	604	NE	ARG	A	887	5.672	51.681	2.476	1.00	32.24	A	N
ATOM	605	CZ	ARG	A	887	4.932	52.523	3.192	1.00	33.92	A	C
ATOM	606	NH1	ARG	A	887	5.124	52.618	4.502	1.00	33.39	A	N
ATOM	607	NH2	ARG	A	887	3.998	53.263	2.597	1.00	33.24	A	N
ATOM	608	C	ARG	A	887	8.138	50.861	−1.644	1.00	23.65	A	C
ATOM	609	O	ARG	A	887	7.051	51.144	−2.140	1.00	24.45	A	O
ATOM	610	N	GLY	A	888	9.291	51.285	−2.150	1.00	24.72	A	N
ATOM	611	CA	GLY	A	888	9.299	52.139	−3.323	1.00	24.04	A	C
ATOM	612	C	GLY	A	888	10.585	52.927	−3.492	1.00	23.39	A	C
ATOM	613	O	GLY	A	888	11.577	52.673	−2.805	1.00	23.48	A	O
ATOM	614	N	VAL	A	889	10.562	53.877	−4.420	1.00	20.54	A	N
ATOM	615	CA	VAL	A	889	11.709	54.719	−4.722	1.00	20.10	A	C
ATOM	616	CB	VAL	A	889	12.123	54.570	−6.200	1.00	21.03	A	C
ATOM	617	CG1	VAL	A	889	13.115	55.656	−6.584	1.00	21.45	A	C
ATOM	618	CG2	VAL	A	889	12.719	53.200	−6.435	1.00	19.77	A	C
ATOM	619	C	VAL	A	889	11.317	56.167	−4.485	1.00	21.40	A	C
ATOM	620	O	VAL	A	889	10.159	56.527	−4.684	1.00	22.69	A	O
ATOM	621	N	SER	A	890	12.262	57.001	−4.057	1.00	20.80	A	N
ATOM	622	CA	SER	A	890	11.952	58.406	−3.830	1.00	22.34	A	C
ATOM	623	CB	SER	A	890	12.629	58.920	−2.556	1.00	21.30	A	C
ATOM	624	OG	SER	A	890	13.977	59.280	−2.804	1.00	24.15	A	O
ATOM	625	C	SER	A	890	12.410	59.250	−5.012	1.00	24.18	A	C
ATOM	626	O	SER	A	890	13.359	58.896	−5.717	1.00	24.15	A	O
ATOM	627	N	TYR	A	891	11.718	60.365	−5.229	1.00	25.30	A	N
ATOM	628	CA	TYR	A	891	12.060	61.284	−6.309	1.00	27.29	A	C
ATOM	629	CB	TYR	A	891	11.002	61.224	−7.411	1.00	27.04	A	C
ATOM	630	CG	TYR	A	891	11.081	59.936	−8.178	1.00	28.70	A	C
ATOM	631	CD1	TYR	A	891	12.162	59.667	−9.000	1.00	29.90	A	C
ATOM	632	CE1	TYR	A	891	12.291	58.455	−9.626	1.00	28.35	A	C
ATOM	633	CD2	TYR	A	891	10.128	58.955	−8.014	1.00	26.81	A	C
ATOM	634	CE2	TYR	A	891	10.248	57.743	−8.632	1.00	27.95	A	C
ATOM	635	CZ	TYR	A	891	11.333	57.491	−9.437	1.00	27.15	A	C
ATOM	636	OH	TYR	A	891	11.482	56.253	−10.028	1.00	25.99	A	O
ATOM	637	C	TYR	A	891	12.236	62.715	−5.803	1.00	27.89	A	C
ATOM	638	O	TYR	A	891	11.358	63.256	−5.136	1.00	28.25	A	O
ATOM	639	N	GLY	A	892	13.384	63.295	−6.149	1.00	29.35	A	N
ATOM	640	CA	GLY	A	892	13.791	64.640	−5.767	1.00	34.56	A	C
ATOM	641	C	GLY	A	892	12.859	65.827	−5.824	1.00	37.08	A	C
ATOM	642	O	GLY	A	892	11.709	65.745	−5.397	1.00	41.32	A	O
ATOM	643	N	PRO	A	893	13.343	66.975	−6.314	1.00	37.48	A	N
ATOM	644	CD	PRO	A	893	12.587	68.245	−6.303	1.00	37.32	A	C
ATOM	645	CA	PRO	A	893	14.706	67.183	−6.804	1.00	37.32	A	C
ATOM	646	CB	PRO	A	893	14.587	68.489	−7.576	1.00	36.43	A	C
ATOM	647	CG	PRO	A	893	13.638	69.267	−6.701	1.00	37.84	A	C
ATOM	648	C	PRO	A	893	15.710	67.298	−5.663	1.00	37.83	A	C
ATOM	649	O	PRO	A	893	15.576	66.660	−4.606	1.00	38.11	A	O
ATOM	650	N	GLY	A	894	16.714	68.134	−5.884	1.00	35.65	A	N
ATOM	651	CA	GLY	A	894	17.725	68.332	−4.865	1.00	33.37	A	C
ATOM	652	C	GLY	A	894	18.628	67.132	−4.686	1.00	30.83	A	C
ATOM	653	O	GLY	A	894	18.401	66.080	−5.272	1.00	29.44	A	O
ATOM	654	N	ARG	A	895	19.654	67.308	−3.861	1.00	31.54	A	N
ATOM	655	CA	ARG	A	895	20.645	66.280	−3.566	1.00	29.64	A	C
ATOM	656	CB	ARG	A	895	21.477	66.703	−2.359	1.00	30.82	A	C
ATOM	657	CG	ARG	A	895	21.949	68.136	−2.436	1.00	36.81	A	C
ATOM	658	CD	ARG	A	895	22.739	68.556	−1.201	1.00	37.21	A	C
ATOM	659	NE	ARG	A	895	23.919	67.725	−1.002	1.00	39.51	A	N
ATOM	660	CZ	ARG	A	895	23.966	66.658	−0.215	1.00	42.26	A	C
ATOM	661	NH1	ARG	A	895	22.885	66.279	0.471	1.00	41.34	A	N
ATOM	662	NH2	ARG	A	895	25.100	65.971	−0.125	1.00	41.86	A	N
ATOM	663	C	ARG	A	895	20.044	64.919	−3.283	1.00	27.07	A	C
ATOM	664	O	ARG	A	895	20.516	63.913	−3.784	1.00	26.22	A	O
ATOM	665	N	GLN	A	896	19.000	64.881	−2.474	1.00	25.66	A	N

TABLE 2-continued

ATOM	666	CA	GLN	A	896	18.418	63.605	−2.141	1.00	26.88	A	C
ATOM	667	CB	GLN	A	896	17.974	63.605	−0.674	1.00	27.75	A	C
ATOM	668	CG	GLN	A	896	19.095	63.703	0.367	1.00	23.25	A	C
ATOM	669	CD	GLN	A	896	18.560	63.532	1.786	1.00	25.71	A	C
ATOM	670	OE1	GLN	A	896	17.686	64.279	2.219	1.00	25.96	A	O
ATOM	671	NE2	GLN	A	896	19.077	62.538	2.511	1.00	24.24	A	N
ATOM	672	C	GLN	A	896	17.253	63.187	−3.041	1.00	28.96	A	C
ATOM	673	O	GLN	A	896	16.220	63.870	−3.113	1.00	32.60	A	O
ATOM	674	N	SER	A	897	17.436	62.056	−3.717	1.00	26.09	A	N
ATOM	675	CA	SER	A	897	16.436	61.488	−4.605	1.00	25.53	A	C
ATOM	676	CB	SER	A	897	16.200	62.418	−5.790	1.00	26.04	A	C
ATOM	677	OG	SER	A	897	15.213	61.887	−6.648	1.00	23.93	A	O
ATOM	678	C	SER	A	897	16.828	60.086	−5.101	1.00	25.24	A	C
ATOM	679	O	SER	A	897	17.987	59.674	−4.993	1.00	22.93	A	O
ATOM	680	N	LEU	A	898	15.856	59.365	−5.656	1.00	24.91	A	N
ATOM	681	CA	LEU	A	898	16.097	58.010	−6.125	1.00	24.03	A	C
ATOM	682	CB	LEU	A	898	17.112	57.998	−7.268	1.00	24.88	A	C
ATOM	683	CG	LEU	A	898	16.549	58.464	−8.609	1.00	23.32	A	C
ATOM	684	CD1	LEU	A	898	17.616	58.439	−9.659	1.00	24.28	A	C
ATOM	685	CD2	LEU	A	898	15.419	57.550	−9.015	1.00	26.25	A	C
ATOM	686	C	LEU	A	898	16.630	57.180	−4.962	1.00	24.34	A	C
ATOM	687	O	LEU	A	898	17.584	56.433	−5.117	1.00	24.06	A	O
ATOM	688	N	ARG	A	899	16.021	57.336	−3.791	1.00	24.15	A	N
ATOM	689	CA	ARG	A	899	16.433	56.589	−2.614	1.00	23.36	A	C
ATOM	690	CB	ARG	A	899	16.396	57.491	−1.376	1.00	22.23	A	C
ATOM	691	CG	ARG	A	899	17.290	58.737	−1.484	1.00	22.55	A	C
ATOM	692	CD	ARG	A	899	17.531	59.430	−0.121	1.00	23.29	A	C
ATOM	693	NE	ARG	A	899	16.342	60.077	0.435	1.00	22.79	A	N
ATOM	694	CZ	ARG	A	899	16.231	60.489	1.698	1.00	23.20	A	C
ATOM	695	NH1	ARG	A	899	15.115	61.066	2.109	1.00	21.75	A	N
ATOM	696	NH2	ARG	A	899	17.226	60.320	2.557	1.00	21.19	A	N
ATOM	697	C	ARG	A	899	15.522	55.370	−2.427	1.00	24.79	A	C
ATOM	698	O	ARG	A	899	14.410	55.313	−2.972	1.00	23.87	A	O
ATOM	699	N	LEU	A	900	16.005	54.395	−1.664	1.00	23.94	A	N
ATOM	700	CA	LEU	A	900	15.258	53.175	−1.425	1.00	23.43	A	C
ATOM	701	CB	LEU	A	900	16.234	51.992	−1.334	1.00	25.73	A	C
ATOM	702	CG	LEU	A	900	17.254	51.879	−2.479	1.00	22.68	A	C
ATOM	703	CD1	LEU	A	900	18.236	50.767	−2.198	1.00	21.83	A	C
ATOM	704	CD2	LEU	A	900	16.513	51.625	−3.782	1.00	23.99	A	C
ATOM	705	C	LEU	A	900	14.467	53.306	−0.134	1.00	23.36	A	C
ATOM	706	O	LEU	A	900	15.055	53.495	0.924	1.00	25.79	A	O
ATOM	707	N	VAL	A	901	13.140	53.215	−0.224	1.00	23.16	A	N
ATOM	708	CA	VAL	A	901	12.247	53.327	0.943	1.00	21.00	A	C
ATOM	709	CB	VAL	A	901	10.967	54.161	0.598	1.00	19.18	A	C
ATOM	710	CG1	VAL	A	901	10.220	54.541	1.872	1.00	16.79	A	C
ATOM	711	CG2	VAL	A	901	11.346	55.412	−0.179	1.00	16.04	A	C
ATOM	712	C	VAL	A	901	11.816	51.921	1.367	1.00	21.72	A	C
ATOM	713	O	VAL	A	901	11.301	51.163	0.550	1.00	20.89	A	O
ATOM	714	N	MET	A	902	12.018	51.573	2.635	1.00	22.44	A	N
ATOM	715	CA	MET	A	902	11.654	50.244	3.133	1.00	22.31	A	C
ATOM	716	CB	MET	A	902	12.914	49.415	3.418	1.00	23.41	A	C
ATOM	717	CG	MET	A	902	14.029	49.527	2.402	1.00	24.33	A	C
ATOM	718	SD	MET	A	902	15.610	48.975	3.107	1.00	28.16	A	S
ATOM	719	CE	MET	A	902	16.470	50.599	3.415	1.00	18.42	A	C
ATOM	720	C	MET	A	902	10.879	50.342	4.445	1.00	22.84	A	C
ATOM	721	O	MET	A	902	10.780	51.417	5.036	1.00	22.65	A	O
ATOM	722	N	GLU	A	903	10.341	49.212	4.901	1.00	23.07	A	N
ATOM	723	CA	GLU	A	903	9.637	49.174	6.175	1.00	24.06	A	C
ATOM	724	CB	GLU	A	903	8.908	47.835	6.369	1.00	21.47	A	C
ATOM	725	CG	GLU	A	903	9.829	46.644	6.571	1.00	25.28	A	C
ATOM	726	CD	GLU	A	903	9.094	45.325	6.793	1.00	25.14	A	C
ATOM	727	OE1	GLU	A	903	8.169	45.267	7.634	1.00	23.48	A	O
ATOM	728	OE2	GLU	A	903	9.458	44.333	6.129	1.00	27.12	A	O
ATOM	729	C	GLU	A	903	10.769	49.342	7.204	1.00	26.12	A	C
ATOM	730	O	GLU	A	903	11.907	48.919	6.962	1.00	25.33	A	O
ATOM	731	N	TYR	A	904	10.465	49.956	8.342	1.00	25.19	A	N
ATOM	732	CA	TYR	A	904	11.480	50.213	9.350	1.00	25.53	A	C
ATOM	733	CB	TYR	A	904	11.375	51.682	9.774	1.00	26.19	A	C
ATOM	734	CG	TYR	A	904	12.144	52.041	11.014	1.00	24.20	A	C
ATOM	735	CD1	TYR	A	904	13.520	51.938	11.052	1.00	23.09	A	C
ATOM	736	CE1	TYR	A	904	14.216	52.277	12.180	1.00	23.97	A	C
ATOM	737	CD2	TYR	A	904	11.489	52.491	12.143	1.00	23.37	A	C
ATOM	738	CE2	TYR	A	904	12.179	52.832	13.273	1.00	23.70	A	C
ATOM	739	CZ	TYR	A	904	13.541	52.728	13.287	1.00	22.96	A	C
ATOM	740	OH	TYR	A	904	14.225	53.123	14.408	1.00	26.04	A	O
ATOM	741	C	TYR	A	904	11.437	49.303	10.576	1.00	25.47	A	C
ATOM	742	O	TYR	A	904	10.451	49.286	11.309	1.00	25.58	A	O
ATOM	743	N	LEU	A	905	12.516	48.553	10.795	1.00	24.91	A	N
ATOM	744	CA	LEU	A	905	12.610	47.649	11.942	1.00	24.94	A	C
ATOM	745	CB	LEU	A	905	13.104	46.273	11.492	1.00	25.49	A	C

TABLE 2-continued

ATOM	746	CG	LEU	A	905	12.069	45.313	10.883	1.00	26.77	A	C
ATOM	747	CD1	LEU	A	905	11.533	45.849	9.540	1.00	22.44	A	C
ATOM	748	CD2	LEU	A	905	12.739	43.934	10.703	1.00	24.93	A	C
ATOM	749	C	LEU	A	905	13.567	48.243	12.977	1.00	24.77	A	C
ATOM	750	O	LEU	A	905	14.774	48.153	12.835	1.00	23.75	A	O
ATOM	751	N	PRO	A	906	13.021	48.844	14.043	1.00	25.08	A	N
ATOM	752	CD	PRO	A	906	11.573	48.801	14.296	1.00	25.48	A	C
ATOM	753	CA	PRO	A	906	13.717	49.499	15.157	1.00	26.75	A	C
ATOM	754	CB	PRO	A	906	12.564	50.077	15.981	1.00	24.51	A	C
ATOM	755	CG	PRO	A	906	11.499	49.097	15.781	1.00	25.37	A	C
ATOM	756	C	PRO	A	906	14.725	48.710	16.010	1.00	27.00	A	C
ATOM	757	O	PRO	A	906	15.696	49.291	16.514	1.00	27.95	A	O
ATOM	758	N	SER	A	907	14.511	47.408	16.171	1.00	26.18	A	N
ATOM	759	CA	SER	A	907	15.424	46.585	16.963	1.00	24.34	A	C
ATOM	760	CB	SER	A	907	14.858	45.187	17.145	1.00	22.15	A	C
ATOM	761	OG	SER	A	907	13.651	45.257	17.880	1.00	24.29	A	O
ATOM	762	C	SER	A	907	16.830	46.503	16.379	1.00	24.51	A	C
ATOM	763	O	SER	A	907	17.781	46.200	17.093	1.00	24.00	A	O
ATOM	764	N	GLY	A	908	16.963	46.765	15.085	1.00	23.26	A	N
ATOM	765	CA	GLY	A	908	18.277	46.751	14.485	1.00	22.85	A	C
ATOM	766	C	GLY	A	908	18.759	45.418	13.965	1.00	23.80	A	C
ATOM	767	O	GLY	A	908	18.047	44.407	14.014	1.00	23.46	A	O
ATOM	768	N	CYS	A	909	19.994	45.425	13.465	1.00	23.36	A	N
ATOM	769	CA	CYS	A	909	20.605	44.232	12.899	1.00	23.89	A	C
ATOM	770	CB	CYS	A	909	21.937	44.568	12.253	1.00	21.36	A	C
ATOM	771	SG	CYS	A	909	23.205	45.003	13.439	1.00	23.09	A	S
ATOM	772	C	CYS	A	909	20.822	43.143	13.931	1.00	24.75	A	C
ATOM	773	O	CYS	A	909	20.742	43.383	15.133	1.00	24.37	A	O
ATOM	774	N	LEU	A	910	21.113	41.943	13.438	1.00	24.76	A	N
ATOM	775	CA	LEU	A	910	21.331	40.788	14.285	1.00	25.40	A	C
ATOM	776	CB	LEU	A	910	21.058	39.497	13.501	1.00	23.11	A	C
ATOM	777	CG	LEU	A	910	21.209	38.168	14.251	1.00	19.95	A	C
ATOM	778	CD1	LEU	A	910	20.317	38.176	15.486	1.00	19.52	A	C
ATOM	779	CD2	LEU	A	910	20.833	37.002	13.331	1.00	17.68	A	C
ATOM	780	C	LEU	A	910	22.761	40.796	14.793	1.00	27.11	A	C
ATOM	781	O	LEU	A	910	23.032	40.324	15.892	1.00	27.00	A	O
ATOM	782	N	ARG	A	911	23.669	41.331	13.983	1.00	28.24	A	N
ATOM	783	CA	ARG	A	911	25.075	41.415	14.352	1.00	28.19	A	C
ATOM	784	CB	ARG	A	911	25.839	42.249	13.316	1.00	28.23	A	C
ATOM	785	CG	ARG	A	911	27.309	42.450	13.625	1.00	30.58	A	C
ATOM	786	CD	ARG	A	911	27.646	43.926	13.789	1.00	33.24	A	C
ATOM	787	NE	ARG	A	911	27.952	44.595	12.524	1.00	36.27	A	N
ATOM	788	CZ	ARG	A	911	27.695	45.878	12.268	1.00	37.56	A	C
ATOM	789	NH1	ARG	A	911	27.115	46.636	13.194	1.00	34.55	A	N
ATOM	790	NH2	ARG	A	911	28.029	46.408	11.090	1.00	36.66	A	N
ATOM	791	C	ARG	A	911	25.205	42.050	15.735	1.00	29.66	A	C
ATOM	792	O	ARG	A	911	25.791	41.461	16.633	1.00	28.96	A	O
ATOM	793	N	ASP	A	912	24.645	43.245	15.911	1.00	30.49	A	N
ATOM	794	CA	ASP	A	912	24.726	43.937	17.198	1.00	31.99	A	C
ATOM	795	CB	ASP	A	912	24.300	45.396	17.041	1.00	31.19	A	C
ATOM	796	CG	ASP	A	912	25.211	46.166	16.109	1.00	35.19	A	C
ATOM	797	OD1	ASP	A	912	24.896	47.327	15.778	1.00	37.95	A	O
ATOM	798	OD2	ASP	A	912	26.251	45.609	15.705	1.00	39.20	A	O
ATOM	799	C	ASP	A	912	23.885	43.274	18.283	1.00	32.12	A	C
ATOM	800	O	ASP	A	912	24.265	43.257	19.454	1.00	33.14	A	O
ATOM	801	N	PHE	A	913	22.744	42.729	17.877	1.00	31.11	A	N
ATOM	802	CA	PHE	A	913	21.818	42.053	18.780	1.00	29.01	A	C
ATOM	803	CB	PHE	A	913	20.610	41.561	17.984	1.00	27.73	A	C
ATOM	804	CG	PHE	A	913	19.543	40.927	18.820	1.00	25.27	A	C
ATOM	805	CD1	PHE	A	913	18.543	41.699	19.380	1.00	25.20	A	C
ATOM	806	CD2	PHE	A	913	19.529	39.559	19.028	1.00	25.36	A	C
ATOM	807	CE1	PHE	A	913	17.544	41.121	20.132	1.00	26.53	A	C
ATOM	808	CE2	PHE	A	913	18.533	38.966	19.783	1.00	27.33	A	C
ATOM	809	CZ	PHE	A	913	17.537	39.749	20.335	1.00	25.91	A	C
ATOM	810	C	PHE	A	913	22.476	40.857	19.472	1.00	29.07	A	C
ATOM	811	O	PHE	A	913	22.295	40.636	20.664	1.00	29.72	A	O
ATOM	812	N	LEU	A	914	23.219	40.074	18.707	1.00	28.66	A	N
ATOM	813	CA	LEU	A	914	23.883	38.910	19.242	1.00	28.77	A	C
ATOM	814	CB	LEU	A	914	24.586	38.145	18.119	1.00	28.26	A	C
ATOM	815	CG	LEU	A	914	23.745	37.401	17.074	1.00	29.50	A	C
ATOM	816	CD1	LEU	A	914	24.598	37.156	15.834	1.00	28.14	A	C
ATOM	817	CD2	LEU	A	914	23.220	36.097	17.634	1.00	25.43	A	C
ATOM	818	C	LEU	A	914	24.910	39.294	20.294	1.00	30.60	A	C
ATOM	819	O	LEU	A	914	25.041	38.616	21.305	1.00	30.77	A	O
ATOM	820	N	GLN	A	915	25.639	40.380	20.057	1.00	31.78	A	N
ATOM	821	CA	GLN	A	915	26.682	40.812	20.986	1.00	32.32	A	C
ATOM	822	CB	GLN	A	915	27.550	41.897	20.346	1.00	29.51	A	C
ATOM	823	CG	GLN	A	915	28.275	41.430	19.105	1.00	27.89	A	C
ATOM	824	CD	GLN	A	915	28.986	42.558	18.381	1.00	30.62	A	C
ATOM	825	OE1	GLN	A	915	29.960	43.110	18.879	1.00	34.44	A	O

TABLE 2-continued

ATOM	826	NE2	GLN	A	915	28.493	42.911	17.201	1.00	32.70	A	N
ATOM	827	C	GLN	A	915	26.147	41.309	22.314	1.00	32.56	A	C
ATOM	828	O	GLN	A	915	26.696	40.998	23.367	1.00	33.01	A	O
ATOM	829	N	ARG	A	916	25.072	42.080	22.259	1.00	35.64	A	N
ATOM	830	CA	ARG	A	916	24.470	42.618	23.466	1.00	38.93	A	C
ATOM	831	CB	ARG	A	916	23.378	43.623	23.111	1.00	40.92	A	C
ATOM	832	CG	ARG	A	916	22.567	44.085	24.316	1.00	46.49	A	C
ATOM	833	CD	ARG	A	916	23.376	45.002	25.246	1.00	51.88	A	C
ATOM	834	NE	ARG	A	916	23.508	46.365	24.717	1.00	55.94	A	N
ATOM	835	CZ	ARG	A	916	22.523	47.263	24.672	1.00	56.13	A	C
ATOM	836	NH1	ARG	A	916	21.311	46.961	25.125	1.00	56.04	A	N
ATOM	837	NH2	ARG	A	916	22.755	48.470	24.171	1.00	56.78	A	N
ATOM	838	C	ARG	A	916	23.880	41.530	24.350	1.00	39.54	A	C
ATOM	839	O	ARG	A	916	24.391	41.269	25.432	1.00	41.77	A	O
ATOM	840	N	HIS	A	917	22.814	40.890	23.881	1.00	40.60	A	N
ATOM	841	CA	HIS	A	917	22.128	39.861	24.657	1.00	40.90	A	C
ATOM	842	CB	HIS	A	917	20.702	39.682	24.144	1.00	41.88	A	C
ATOM	843	CG	HIS	A	917	20.000	40.970	23.863	1.00	43.18	A	C
ATOM	844	CD2	HIS	A	917	19.191	41.736	24.632	1.00	43.95	A	C
ATOM	845	ND1	HIS	A	917	20.124	41.635	22.660	1.00	43.84	A	N
ATOM	846	CE1	HIS	A	917	19.421	42.750	22.702	1.00	45.33	A	C
ATOM	847	NE2	HIS	A	917	18.844	42.838	23.889	1.00	45.00	A	N
ATOM	848	C	HIS	A	917	22.801	38.506	24.677	1.00	40.71	A	C
ATOM	849	O	HIS	A	917	22.189	37.520	25.080	1.00	40.37	A	O
ATOM	850	N	ARG	A	918	24.054	38.451	24.249	1.00	41.70	A	N
ATOM	851	CA	ARG	A	918	24.784	37.193	24.222	1.00	43.37	A	C
ATOM	852	CB	ARG	A	918	26.288	37.459	24.141	1.00	44.88	A	C
ATOM	853	CG	ARG	A	918	27.124	36.231	23.793	1.00	46.33	A	C
ATOM	854	CD	ARG	A	918	28.607	36.535	23.906	1.00	48.49	A	C
ATOM	855	NE	ARG	A	918	29.442	35.414	23.485	1.00	51.68	A	N
ATOM	856	CZ	ARG	A	918	29.319	34.174	23.942	1.00	53.95	A	C
ATOM	857	NH1	ARG	A	918	28.386	33.879	24.840	1.00	55.47	A	N
ATOM	858	NH2	ARG	A	918	30.137	33.228	23.502	1.00	55.10	A	N
ATOM	859	C	ARG	A	918	24.471	36.386	25.476	1.00	44.88	A	C
ATOM	860	O	ARG	A	918	24.252	35.176	25.416	1.00	45.56	A	O
ATOM	861	N	ALA	A	919	24.436	37.078	26.610	1.00	46.35	A	N
ATOM	862	CA	ALA	A	919	24.164	36.459	27.900	1.00	46.62	A	C
ATOM	863	CB	ALA	A	919	23.801	37.532	28.904	1.00	46.80	A	C
ATOM	864	C	ALA	A	919	23.082	35.375	27.886	1.00	46.74	A	C
ATOM	865	O	ALA	A	919	23.342	34.226	28.242	1.00	45.80	A	O
ATOM	866	N	ARG	A	920	21.871	35.737	27.477	1.00	46.25	A	N
ATOM	867	CA	ARG	A	920	20.774	34.780	27.457	1.00	46.08	A	C
ATOM	868	CB	ARG	A	920	19.622	35.308	28.316	1.00	47.54	A	C
ATOM	869	CG	ARG	A	920	19.363	36.807	28.203	1.00	47.40	A	C
ATOM	870	CD	ARG	A	920	18.610	37.168	26.940	1.00	49.45	A	C
ATOM	871	NE	ARG	A	920	18.194	38.569	26.925	1.00	49.65	A	N
ATOM	872	CZ	ARG	A	920	17.400	39.098	26.001	1.00	49.78	A	C
ATOM	873	NH1	ARG	A	920	16.933	38.342	25.013	1.00	49.39	A	N
ATOM	874	NH2	ARG	A	920	17.069	40.379	26.067	1.00	49.52	A	N
ATOM	875	C	ARG	A	920	20.261	34.405	26.074	1.00	46.13	A	C
ATOM	876	O	ARG	A	920	19.134	34.750	25.705	1.00	44.96	A	O
ATOM	877	N	LEU	A	921	21.085	33.678	25.322	1.00	45.06	A	N
ATOM	878	CA	LEU	A	921	20.727	33.241	23.973	1.00	44.84	A	C
ATOM	879	CB	LEU	A	921	21.149	34.290	22.942	1.00	44.96	A	C
ATOM	880	CG	LEU	A	921	20.422	35.635	22.925	1.00	45.84	A	C
ATOM	881	CD1	LEU	A	921	21.093	36.550	21.892	1.00	45.14	A	C
ATOM	882	CD2	LEU	A	921	18.940	35.427	22.594	1.00	45.08	A	C
ATOM	883	C	LEU	A	921	21.401	31.922	23.639	1.00	44.13	A	C
ATOM	884	O	LEU	A	921	22.491	31.906	23.071	1.00	44.16	A	O
ATOM	885	N	ASP	A	922	20.749	30.816	23.980	1.00	43.31	A	N
ATOM	886	CA	ASP	A	922	21.317	29.496	23.720	1.00	42.52	A	C
ATOM	887	CB	ASP	A	922	20.505	28.420	24.443	1.00	42.97	A	C
ATOM	888	CG	ASP	A	922	19.069	28.384	23.995	1.00	42.64	A	C
ATOM	889	OD1	ASP	A	922	18.842	28.390	22.772	1.00	43.81	A	O
ATOM	890	OD2	ASP	A	922	18.169	28.341	24.857	1.00	43.17	A	O
ATOM	891	C	ASP	A	922	21.418	29.150	22.235	1.00	40.48	A	C
ATOM	892	O	ASP	A	922	21.060	29.945	21.377	1.00	41.42	A	O
ATOM	893	N	ALA	A	923	21.896	27.947	21.942	1.00	38.52	A	N
ATOM	894	CA	ALA	A	923	22.068	27.495	20.565	1.00	36.73	A	C
ATOM	895	CB	ALA	A	923	22.890	26.215	20.546	1.00	36.05	A	C
ATOM	896	C	ALA	A	923	20.743	27.273	19.839	1.00	36.44	A	C
ATOM	897	O	ALA	A	923	20.691	27.246	18.610	1.00	35.30	A	O
ATOM	898	N	SER	A	924	19.675	27.103	20.604	1.00	35.48	A	N
ATOM	899	CA	SER	A	924	18.371	26.892	20.010	1.00	35.00	A	C
ATOM	900	CB	SER	A	924	17.343	26.562	21.095	1.00	34.87	A	C
ATOM	901	OG	SER	A	924	17.551	25.248	21.574	1.00	36.69	A	O
ATOM	902	C	SER	A	924	17.954	28.144	19.256	1.00	33.85	A	C
ATOM	903	O	SER	A	924	17.547	28.087	18.095	1.00	33.17	A	O
ATOM	904	N	ARG	A	925	18.067	29.276	19.931	1.00	32.59	A	N
ATOM	905	CA	ARG	A	925	17.707	30.548	19.348	1.00	32.54	A	C

TABLE 2-continued

ATOM	906	CB	ARG	A	925	17.974	31.663	20.364	1.00	33.17	A	C
ATOM	907	CG	ARG	A	925	17.325	32.978	20.013	1.00	36.60	A	C
ATOM	908	CD	ARG	A	925	16.015	33.157	20.747	1.00	39.24	A	C
ATOM	909	NE	ARG	A	925	15.178	31.964	20.685	1.00	42.43	A	N
ATOM	910	CZ	ARG	A	925	13.937	31.905	21.157	1.00	42.81	A	C
ATOM	911	NH1	ARG	A	925	13.237	30.779	21.073	1.00	43.91	A	N
ATOM	912	NH2	ARG	A	925	13.391	32.983	21.699	1.00	41.57	A	N
ATOM	913	C	ARG	A	925	18.522	30.776	18.066	1.00	31.35	A	C
ATOM	914	O	ARG	A	925	17.989	31.220	17.045	1.00	30.98	A	O
ATOM	915	N	LEU	A	926	19.812	30.461	18.123	1.00	29.39	A	N
ATOM	916	CA	LEU	A	926	20.684	30.645	16.968	1.00	26.98	A	C
ATOM	917	CB	LEU	A	926	22.137	30.278	17.321	1.00	25.24	A	C
ATOM	918	CG	LEU	A	926	22.729	30.922	18.586	1.00	26.47	A	C
ATOM	919	CD1	LEU	A	926	24.164	30.453	18.762	1.00	22.76	A	C
ATOM	920	CD2	LEU	A	926	22.660	32.470	18.498	1.00	23.66	A	C
ATOM	921	C	LEU	A	926	20.177	29.759	15.835	1.00	25.57	A	C
ATOM	922	O	LEU	A	926	20.222	30.144	14.674	1.00	25.52	A	O
ATOM	923	N	LEU	A	927	19.695	28.573	16.185	1.00	24.45	A	N
ATOM	924	CA	LEU	A	927	19.166	27.636	15.203	1.00	25.10	A	C
ATOM	925	CB	LEU	A	927	18.913	26.276	15.860	1.00	23.29	A	C
ATOM	926	CG	LEU	A	927	20.192	25.452	16.079	1.00	23.60	A	C
ATOM	927	CD1	LEU	A	927	19.914	24.230	16.951	1.00	21.29	A	C
ATOM	928	CD2	LEU	A	927	20.741	25.045	14.713	1.00	21.28	A	C
ATOM	929	C	LEU	A	927	17.881	28.176	14.579	1.00	25.54	A	C
ATOM	930	O	LEU	A	927	17.653	28.021	13.387	1.00	27.60	A	O
ATOM	931	N	LEU	A	928	17.043	28.813	15.382	1.00	26.21	A	N
ATOM	932	CA	LEU	A	928	15.817	29.377	14.860	1.00	28.46	A	C
ATOM	933	CB	LEU	A	928	14.986	29.994	15.990	1.00	29.01	A	C
ATOM	934	CG	LEU	A	928	13.640	30.609	15.580	1.00	30.63	A	C
ATOM	935	CD1	LEU	A	928	12.726	29.543	14.983	1.00	28.56	A	C
ATOM	936	CD2	LEU	A	928	12.984	31.247	16.798	1.00	30.31	A	C
ATOM	937	C	LEU	A	928	16.172	30.452	13.829	1.00	28.78	A	C
ATOM	938	O	LEU	A	928	15.627	30.467	12.727	1.00	31.05	A	O
ATOM	939	N	TYR	A	929	17.092	31.345	14.188	1.00	28.81	A	N
ATOM	940	CA	TYR	A	929	17.499	32.404	13.278	1.00	26.06	A	C
ATOM	941	CB	TYR	A	929	18.554	33.313	13.917	1.00	24.85	A	C
ATOM	942	CG	TYR	A	929	18.091	34.038	15.171	1.00	24.20	A	C
ATOM	943	CD1	TYR	A	929	16.739	34.249	15.420	1.00	22.44	A	C
ATOM	944	CE1	TYR	A	929	16.319	34.898	16.562	1.00	23.86	A	C
ATOM	945	CD2	TYR	A	929	19.014	34.512	16.108	1.00	24.65	A	C
ATOM	946	CE2	TYR	A	929	18.600	35.165	17.251	1.00	23.64	A	C
ATOM	947	CZ	TYR	A	929	17.255	35.352	17.476	1.00	23.72	A	C
ATOM	948	OH	TYR	A	929	16.836	35.970	18.627	1.00	26.16	A	O
ATOM	949	C	TYR	A	929	18.068	31.765	12.032	1.00	25.81	A	C
ATOM	950	O	TYR	A	929	17.813	32.217	10.924	1.00	26.45	A	O
ATOM	951	N	SER	A	930	18.843	30.707	12.208	1.00	25.98	A	N
ATOM	952	CA	SER	A	930	19.426	30.035	11.059	1.00	27.82	A	C
ATOM	953	CB	SER	A	930	20.325	28.885	11.513	1.00	28.75	A	C
ATOM	954	OG	SER	A	930	21.528	29.393	12.064	1.00	30.14	A	O
ATOM	955	C	SER	A	930	18.360	29.507	10.111	1.00	28.13	A	C
ATOM	956	O	SER	A	930	18.482	29.628	8.886	1.00	27.24	A	O
ATOM	957	N	SER	A	931	17.313	28.932	10.694	1.00	27.11	A	N
ATOM	958	CA	SER	A	931	16.211	28.360	9.934	1.00	25.57	A	C
ATOM	959	CB	SER	A	931	15.262	27.618	10.887	1.00	25.40	A	C
ATOM	960	OG	SER	A	931	14.196	26.996	10.183	1.00	26.62	A	O
ATOM	961	C	SER	A	931	15.446	29.432	9.148	1.00	23.59	A	C
ATOM	962	O	SER	A	931	15.193	29.284	7.957	1.00	21.65	A	O
ATOM	963	N	GLN	A	932	15.089	30.515	9.821	1.00	21.56	A	N
ATOM	964	CA	GLN	A	932	14.340	31.578	9.173	1.00	20.32	A	C
ATOM	965	CB	GLN	A	932	13.915	32.619	10.197	1.00	19.20	A	C
ATOM	966	CG	GLN	A	932	13.032	32.067	11.272	1.00	13.20	A	C
ATOM	967	CD	GLN	A	932	12.775	33.085	12.345	1.00	17.11	A	C
ATOM	968	OE1	GLN	A	932	13.518	34.061	12.478	1.00	19.07	A	O
ATOM	969	NE2	GLN	A	932	11.730	32.864	13.136	1.00	18.46	A	N
ATOM	970	C	GLN	A	932	15.146	32.228	8.066	1.00	19.98	A	C
ATOM	971	O	GLN	A	932	14.611	32.482	7.004	1.00	20.76	A	O
ATOM	972	N	ILE	A	933	16.430	32.487	8.304	1.00	19.95	A	N
ATOM	973	CA	ILE	A	933	17.294	33.088	7.287	1.00	19.59	A	C
ATOM	974	CB	ILE	A	933	18.744	33.298	7.834	1.00	16.81	A	C
ATOM	975	CG2	ILE	A	933	19.716	33.611	6.700	1.00	13.19	A	C
ATOM	976	CG1	ILE	A	933	18.747	34.420	8.876	1.00	14.44	A	C
ATOM	977	CD1	ILE	A	933	19.937	34.392	9.822	1.00	10.84	A	C
ATOM	978	C	ILE	A	933	17.336	32.167	6.067	1.00	21.91	A	C
ATOM	979	O	ILE	A	933	17.282	32.635	4.931	1.00	24.84	A	O
ATOM	980	N	CYS	A	934	17.422	30.858	6.302	1.00	22.23	A	N
ATOM	981	CA	CYS	A	934	17.471	29.894	5.201	1.00	23.32	A	C
ATOM	982	CB	CYS	A	934	17.708	28.471	5.715	1.00	21.69	A	C
ATOM	983	SG	CYS	A	934	18.292	27.313	4.412	1.00	30.12	A	S
ATOM	984	C	CYS	A	934	16.174	29.912	4.401	1.00	23.55	A	C
ATOM	985	O	CYS	A	934	16.186	29.820	3.181	1.00	22.75	A	O

TABLE 2-continued

ATOM	986	N	LYS	A	935	15.053	30.005	5.101	1.00	25.04	A	N
ATOM	987	CA	LYS	A	935	13.758	30.047	4.447	1.00	26.11	A	C
ATOM	988	CB	LYS	A	935	12.641	30.114	5.487	1.00	28.76	A	C
ATOM	989	CG	LYS	A	935	12.201	28.770	5.994	1.00	30.78	A	C
ATOM	990	CD	LYS	A	935	11.682	27.924	4.849	1.00	37.03	A	C
ATOM	991	CE	LYS	A	935	10.571	28.633	4.079	1.00	38.59	A	C
ATOM	992	NZ	LYS	A	935	9.503	29.151	4.978	1.00	39.74	A	N
ATOM	993	C	LYS	A	935	13.684	31.280	3.558	1.00	25.61	A	C
ATOM	994	O	LYS	A	935	13.192	31.218	2.432	1.00	25.18	A	O
ATOM	995	N	GLY	A	936	14.184	32.401	4.063	1.00	23.46	A	N
ATOM	996	CA	GLY	A	936	14.139	33.625	3.288	1.00	25.18	A	C
ATOM	997	C	GLY	A	936	14.925	33.529	1.997	1.00	25.97	A	C
ATOM	998	O	GLY	A	936	14.438	33.854	0.910	1.00	25.47	A	O
ATOM	999	N	MET	A	937	16.160	33.068	2.122	1.00	25.86	A	N
ATOM	1000	CA	MET	A	937	17.025	32.935	0.968	1.00	25.43	A	C
ATOM	1001	CB	MET	A	937	18.398	32.465	1.415	1.00	21.83	A	C
ATOM	1002	CG	MET	A	937	19.145	33.521	2.195	1.00	22.95	A	C
ATOM	1003	SD	MET	A	937	19.251	35.048	1.253	1.00	19.04	A	S
ATOM	1004	CE	MET	A	937	20.391	34.539	0.040	1.00	19.63	A	C
ATOM	1005	C	MET	A	937	16.452	31.990	−0.070	1.00	25.93	A	C
ATOM	1006	O	MET	A	937	16.563	32.247	−1.269	1.00	25.39	A	O
ATOM	1007	N	GLU	A	938	15.844	30.898	0.396	1.00	25.81	A	N
ATOM	1008	CA	GLU	A	938	15.249	29.907	−0.492	1.00	28.06	A	C
ATOM	1009	CB	GLU	A	938	14.692	28.711	0.305	1.00	29.00	A	C
ATOM	1010	CG	GLU	A	938	13.949	27.709	−0.573	1.00	34.20	A	C
ATOM	1011	CD	GLU	A	938	12.966	26.819	0.187	1.00	37.81	A	C
ATOM	1012	OE1	GLU	A	938	12.368	27.286	1.189	1.00	41.55	A	O
ATOM	1013	OE2	GLU	A	938	12.781	25.653	−0.234	1.00	37.20	A	O
ATOM	1014	C	GLU	A	938	14.129	30.559	−1.309	1.00	28.74	A	C
ATOM	1015	O	GLU	A	938	14.013	30.344	−2.513	1.00	27.91	A	O
ATOM	1016	N	TYR	A	939	13.304	31.358	−0.647	1.00	28.43	A	N
ATOM	1017	CA	TYR	A	939	12.232	32.039	−1.341	1.00	27.01	A	C
ATOM	1018	CB	TYR	A	939	11.367	32.814	−0.346	1.00	27.10	A	C
ATOM	1019	CG	TYR	A	939	10.389	33.739	−1.025	1.00	26.91	A	C
ATOM	1020	CD1	TYR	A	939	9.233	33.245	−1.631	1.00	25.87	A	C
ATOM	1021	CE1	TYR	A	939	8.373	34.090	−2.330	1.00	25.22	A	C
ATOM	1022	CD2	TYR	A	939	10.654	35.101	−1.130	1.00	26.73	A	C
ATOM	1023	CE2	TYR	A	939	9.803	35.946	−1.825	1.00	26.34	A	C
ATOM	1024	CZ	TYR	A	939	8.671	35.436	−2.424	1.00	25.07	A	C
ATOM	1025	OH	TYR	A	939	7.873	36.269	−3.156	1.00	24.42	A	O
ATOM	1026	C	TYR	A	939	12.823	33.007	−2.377	1.00	27.57	A	C
ATOM	1027	O	TYR	A	939	12.354	33.085	−3.515	1.00	27.74	A	O
ATOM	1028	N	LEU	A	940	13.865	33.739	−1.986	1.00	27.06	A	N
ATOM	1029	CA	LEU	A	940	14.483	34.697	−2.892	1.00	25.89	A	C
ATOM	1030	CB	LEU	A	940	15.561	35.505	−2.160	1.00	25.81	A	C
ATOM	1031	CG	LEU	A	940	15.134	36.223	−0.866	1.00	27.33	A	C
ATOM	1032	CD1	LEU	A	940	16.214	37.236	−0.463	1.00	25.01	A	C
ATOM	1033	CD2	LEU	A	940	13.807	36.937	−1.051	1.00	25.43	A	C
ATOM	1034	C	LEU	A	940	15.057	34.002	−4.126	1.00	26.08	A	C
ATOM	1035	O	LEU	A	940	14.907	34.479	−5.252	1.00	26.56	A	O
ATOM	1036	N	GLY	A	941	15.707	32.865	−3.924	1.00	26.30	A	N
ATOM	1037	CA	GLY	A	941	16.246	32.138	−5.062	1.00	25.14	A	C
ATOM	1038	C	GLY	A	941	15.156	31.632	−6.004	1.00	23.69	A	C
ATOM	1039	O	GLY	A	941	15.274	31.741	−7.223	1.00	21.15	A	O
ATOM	1040	N	SER	A	942	14.079	31.089	−5.452	1.00	22.19	A	N
ATOM	1041	CA	SER	A	942	13.019	30.577	−6.306	1.00	24.17	A	C
ATOM	1042	CB	SER	A	942	11.900	29.952	−5.468	1.00	21.56	A	C
ATOM	1043	OG	SER	A	942	11.195	30.924	−4.706	1.00	21.92	A	O
ATOM	1044	C	SER	A	942	12.452	31.681	−7.199	1.00	26.30	A	C
ATOM	1045	O	SER	A	942	11.878	31.406	−8.257	1.00	27.98	A	O
ATOM	1046	N	ARG	A	943	12.623	32.928	−6.776	1.00	24.94	A	N
ATOM	1047	CA	ARG	A	943	12.117	34.059	−7.535	1.00	25.38	A	C
ATOM	1048	CB	ARG	A	943	11.431	35.055	−6.597	1.00	26.85	A	C
ATOM	1049	CG	ARG	A	943	10.155	34.526	−5.972	1.00	28.29	A	C
ATOM	1050	CD	ARG	A	943	9.079	34.335	−7.038	1.00	34.65	A	C
ATOM	1051	NE	ARG	A	943	7.827	33.831	−6.480	1.00	35.43	A	N
ATOM	1052	CZ	ARG	A	943	7.681	32.630	−5.926	1.00	37.49	A	C
ATOM	1053	NH1	ARG	A	943	6.501	32.258	−5.435	1.00	36.56	A	N
ATOM	1054	NH2	ARG	A	943	8.710	31.794	−5.871	1.00	36.84	A	N
ATOM	1055	C	ARG	A	943	13.247	34.734	−8.300	1.00	25.91	A	C
ATOM	1056	O	ARG	A	943	13.121	35.867	−8.767	1.00	25.66	A	O
ATOM	1057	N	ARG	A	944	14.356	34.015	−8.425	1.00	27.92	A	N
ATOM	1058	CA	ARG	A	944	15.539	34.497	−9.140	1.00	28.02	A	C
ATOM	1059	CB	ARG	A	944	15.225	34.609	−10.633	1.00	29.49	A	C
ATOM	1060	CG	ARG	A	944	14.771	33.282	−11.235	1.00	33.87	A	C
ATOM	1061	CD	ARG	A	944	14.640	33.361	−12.738	1.00	38.79	A	C
ATOM	1062	NE	ARG	A	944	13.924	32.213	−13.289	1.00	41.68	A	N
ATOM	1063	CZ	ARG	A	944	14.406	30.977	−13.353	1.00	42.92	A	C
ATOM	1064	NH1	ARG	A	944	15.622	30.700	−12.903	1.00	44.38	A	N
ATOM	1065	NH2	ARG	A	944	13.660	30.010	−13.865	1.00	43.95	A	N

TABLE 2-continued

ATOM	1066	C	ARG	A	944	16.134	35.806	−8.616	1.00	26.36	A	C
ATOM	1067	O	ARG	A	944	16.580	36.652	−9.380	1.00	27.18	A	O
ATOM	1068	N	CYS	A	945	16.158	35.957	−7.300	1.00	25.76	A	N
ATOM	1069	CA	CYS	A	945	16.715	37.152	−6.691	1.00	25.68	A	C
ATOM	1070	CB	CYS	A	945	15.708	37.756	−5.711	1.00	26.82	A	C
ATOM	1071	SG	CYS	A	945	16.350	39.138	−4.735	1.00	32.67	A	S
ATOM	1072	C	CYS	A	945	18.009	36.812	−5.951	1.00	23.68	A	C
ATOM	1073	O	CYS	A	945	18.003	36.003	−5.029	1.00	21.55	A	O
ATOM	1074	N	VAL	A	946	19.107	37.434	−6.369	1.00	22.39	A	N
ATOM	1075	CA	VAL	A	946	20.421	37.242	−5.748	1.00	22.12	A	C
ATOM	1076	CB	VAL	A	946	21.531	37.211	−6.820	1.00	20.56	A	C
ATOM	1077	CG1	VAL	A	946	22.898	37.089	−6.167	1.00	19.82	A	C
ATOM	1078	CG2	VAL	A	946	21.296	36.053	−7.757	1.00	18.31	A	C
ATOM	1079	C	VAL	A	946	20.699	38.396	−4.777	1.00	22.09	A	C
ATOM	1080	O	VAL	A	946	20.579	39.568	−5.152	1.00	25.08	A	O
ATOM	1081	N	HIS	A	947	21.070	38.058	−3.544	1.00	21.72	A	N
ATOM	1082	CA	HIS	A	947	21.360	39.037	−2.485	1.00	23.37	A	C
ATOM	1083	CB	HIS	A	947	21.438	38.345	−1.118	1.00	21.69	A	C
ATOM	1084	CG	HIS	A	947	21.439	39.299	0.036	1.00	20.53	A	C
ATOM	1085	CD2	HIS	A	947	22.147	40.432	0.263	1.00	17.46	A	C
ATOM	1086	ND1	HIS	A	947	20.554	39.183	1.088	1.00	16.91	A	N
ATOM	1087	CE1	HIS	A	947	20.710	40.208	1.903	1.00	15.92	A	C
ATOM	1088	NE2	HIS	A	947	21.669	40.982	1.427	1.00	17.07	A	N
ATOM	1089	C	HIS	A	947	22.657	39.792	−2.706	1.00	24.97	A	C
ATOM	1090	O	HIS	A	947	22.679	41.018	−2.693	1.00	27.85	A	O
ATOM	1091	N	ARG	A	948	23.741	39.051	−2.887	1.00	28.00	A	N
ATOM	1092	CA	ARG	A	948	25.065	39.629	−3.127	1.00	31.02	A	C
ATOM	1093	CB	ARG	A	948	25.015	40.688	−4.243	1.00	32.92	A	C
ATOM	1094	CG	ARG	A	948	26.344	41.444	−4.373	1.00	38.57	A	C
ATOM	1095	CD	ARG	A	948	26.349	42.551	−5.425	1.00	41.31	A	C
ATOM	1096	NE	ARG	A	948	27.434	43.507	−5.196	1.00	42.45	A	N
ATOM	1097	CZ	ARG	A	948	27.956	44.285	−6.138	1.00	47.28	A	C
ATOM	1098	NH1	ARG	A	948	28.936	45.129	−5.838	1.00	48.64	A	N
ATOM	1099	NH2	ARG	A	948	27.505	44.210	−7.384	1.00	48.13	A	N
ATOM	1100	C	ARG	A	948	25.797	40.218	−1.912	1.00	30.74	A	C
ATOM	1101	O	ARG	A	948	27.021	40.378	−1.951	1.00	32.58	A	O
ATOM	1102	N	ASP	A	949	25.080	40.531	−0.836	1.00	28.19	A	N
ATOM	1103	CA	ASP	A	949	25.741	41.085	0.347	1.00	25.95	A	C
ATOM	1104	CB	ASP	A	949	25.628	42.611	0.325	1.00	28.52	A	C
ATOM	1105	CG	ASP	A	949	26.488	43.282	1.373	1.00	29.95	A	C
ATOM	1106	OD1	ASP	A	949	27.589	42.767	1.656	1.00	29.48	A	O
ATOM	1107	OD2	ASP	A	949	26.069	44.339	1.899	1.00	29.30	A	O
ATOM	1108	C	ASP	A	949	25.110	40.515	1.613	1.00	24.72	A	C
ATOM	1109	O	ASP	A	949	24.730	41.245	2.522	1.00	21.62	A	O
ATOM	1110	N	LEU	A	950	25.006	39.194	1.672	1.00	23.77	A	N
ATOM	1111	CA	LEU	A	950	24.383	38.558	2.822	1.00	22.86	A	C
ATOM	1112	CB	LEU	A	950	23.932	37.141	2.451	1.00	19.95	A	C
ATOM	1113	CG	LEU	A	950	23.108	36.364	3.482	1.00	20.83	A	C
ATOM	1114	CD1	LEU	A	950	21.733	37.032	3.667	1.00	15.52	A	C
ATOM	1115	CD2	LEU	A	950	22.938	34.917	3.005	1.00	17.15	A	C
ATOM	1116	C	LEU	A	950	25.370	38.529	3.979	1.00	21.92	A	C
ATOM	1117	O	LEU	A	950	26.556	38.301	3.781	1.00	19.70	A	O
ATOM	1118	N	ALA	A	951	24.876	38.762	5.189	1.00	21.14	A	N
ATOM	1119	CA	ALA	A	951	25.740	38.768	6.358	1.00	19.64	A	C
ATOM	1120	CB	ALA	A	951	26.860	39.772	6.165	1.00	16.06	A	C
ATOM	1121	C	ALA	A	951	24.917	39.115	7.585	1.00	21.41	A	C
ATOM	1122	O	ALA	A	951	23.812	39.664	7.475	1.00	23.99	A	O
ATOM	1123	N	ALA	A	952	25.447	38.796	8.760	1.00	21.05	A	N
ATOM	1124	CA	ALA	A	952	24.729	39.063	10.002	1.00	19.39	A	C
ATOM	1125	CB	ALA	A	952	25.569	38.616	11.205	1.00	18.53	A	C
ATOM	1126	C	ALA	A	952	24.325	40.532	10.137	1.00	18.69	A	C
ATOM	1127	O	ALA	A	952	23.322	40.844	10.772	1.00	21.48	A	O
ATOM	1128	N	ARG	A	953	25.114	41.440	9.570	1.00	17.77	A	N
ATOM	1129	CA	ARG	A	953	24.757	42.854	9.618	1.00	19.31	A	C
ATOM	1130	CB	ARG	A	953	25.922	43.735	9.171	1.00	17.94	A	C
ATOM	1131	CG	ARG	A	953	26.277	43.580	7.723	1.00	16.54	A	C
ATOM	1132	CD	ARG	A	953	27.394	44.538	7.370	1.00	18.36	A	C
ATOM	1133	NE	ARG	A	953	28.034	44.230	6.088	1.00	20.26	A	N
ATOM	1134	CZ	ARG	A	953	28.894	43.232	5.895	1.00	18.10	A	C
ATOM	1135	NH1	ARG	A	953	29.222	42.432	6.902	1.00	22.15	A	N
ATOM	1136	NH2	ARG	A	953	29.437	43.039	4.703	1.00	14.98	A	N
ATOM	1137	C	ARG	A	953	23.551	43.142	8.704	1.00	20.52	A	C
ATOM	1138	O	ARG	A	953	22.786	44.069	8.955	1.00	19.49	A	O
ATOM	1139	N	ASN	A	954	23.384	42.376	7.629	1.00	20.55	A	N
ATOM	1140	CA	ASN	A	954	22.235	42.638	6.768	1.00	22.29	A	C
ATOM	1141	CB	ASN	A	954	22.614	42.519	5.274	1.00	18.54	A	C
ATOM	1142	CG	ASN	A	954	23.351	43.761	4.753	1.00	17.79	A	C
ATOM	1143	OD1	ASN	A	954	23.022	44.875	5.122	1.00	19.98	A	O
ATOM	1144	ND2	ASN	A	954	24.335	43.566	3.889	1.00	17.35	A	N
ATOM	1145	C	ASN	A	954	21.022	41.759	7.124	1.00	22.75	A	C

TABLE 2-continued

ATOM	1146	O	ASN	A	954	20.183	41.472	6.279	1.00	23.62	A	O
ATOM	1147	N	ILE	A	955	20.952	41.339	8.389	1.00	24.09	A	N
ATOM	1148	CA	ILE	A	955	19.837	40.533	8.902	1.00	23.45	A	C
ATOM	1149	CB	ILE	A	955	20.306	39.205	9.575	1.00	23.56	A	C
ATOM	1150	CG2	ILE	A	955	19.135	38.562	10.335	1.00	22.40	A	C
ATOM	1151	CG1	ILE	A	955	20.812	38.215	8.527	1.00	22.88	A	C
ATOM	1152	CD1	ILE	A	955	19.716	37.621	7.691	1.00	21.73	A	C
ATOM	1153	C	ILE	A	955	19.211	41.390	9.988	1.00	24.33	A	C
ATOM	1154	O	ILE	A	955	19.818	41.580	11.038	1.00	25.58	A	O
ATOM	1155	N	LEU	A	956	18.014	41.917	9.737	1.00	25.10	A	N
ATOM	1156	CA	LEU	A	956	17.326	42.762	10.712	1.00	23.60	A	C
ATOM	1157	CB	LEU	A	956	16.487	43.821	9.990	1.00	20.79	A	C
ATOM	1158	CG	LEU	A	956	17.271	44.953	9.322	1.00	19.09	A	C
ATOM	1159	CD1	LEU	A	956	16.344	45.759	8.426	1.00	15.72	A	C
ATOM	1160	CD2	LEU	A	956	17.901	45.843	10.386	1.00	16.65	A	C
ATOM	1161	C	LEU	A	956	16.446	41.944	11.655	1.00	25.28	A	C
ATOM	1162	O	LEU	A	956	15.913	40.893	11.282	1.00	27.16	A	O
ATOM	1163	N	VAL	A	957	16.301	42.441	12.880	1.00	24.88	A	N
ATOM	1164	CA	VAL	A	957	15.505	41.773	13.902	1.00	24.09	A	C
ATOM	1165	CB	VAL	A	957	16.188	41.866	15.313	1.00	23.67	A	C
ATOM	1166	CG1	VAL	A	957	15.218	41.439	16.419	1.00	18.34	A	C
ATOM	1167	CG2	VAL	A	957	17.431	40.979	15.346	1.00	22.54	A	C
ATOM	1168	C	VAL	A	957	14.093	42.329	14.006	1.00	24.66	A	C
ATOM	1169	O	VAL	A	957	13.885	43.510	14.288	1.00	23.71	A	O
ATOM	1170	N	GLU	A	958	13.125	41.456	13.761	1.00	25.24	A	N
ATOM	1171	CA	GLU	A	958	11.729	41.821	13.842	1.00	27.40	A	C
ATOM	1172	CB	GLU	A	958	10.877	40.821	13.061	1.00	27.40	A	C
ATOM	1173	CG	GLU	A	958	9.407	40.926	13.373	1.00	29.36	A	C
ATOM	1174	CD	GLU	A	958	8.805	42.206	12.865	1.00	30.52	A	C
ATOM	1175	OE1	GLU	A	958	7.699	42.558	13.321	1.00	33.77	A	O
ATOM	1176	OE2	GLU	A	958	9.432	42.856	12.001	1.00	34.54	A	O
ATOM	1177	C	GLU	A	958	11.380	41.769	15.324	1.00	27.35	A	C
ATOM	1178	O	GLU	A	958	10.733	42.669	15.855	1.00	29.14	A	O
ATOM	1179	N	SER	A	959	11.822	40.704	15.982	1.00	28.13	A	N
ATOM	1180	CA	SER	A	959	11.598	40.519	17.409	1.00	29.62	A	C
ATOM	1181	CB	SER	A	959	10.139	40.162	17.700	1.00	27.47	A	C
ATOM	1182	OG	SER	A	959	9.899	38.786	17.467	1.00	27.72	A	O
ATOM	1183	C	SER	A	959	12.514	39.388	17.873	1.00	32.26	A	C
ATOM	1184	O	SER	A	959	13.239	38.808	17.071	1.00	31.08	A	O
ATOM	1185	N	GLU	A	960	12.474	39.083	19.168	1.00	34.51	A	N
ATOM	1186	CA	GLU	A	960	13.304	38.041	19.755	1.00	35.90	A	C
ATOM	1187	CB	GLU	A	960	12.896	37.807	21.208	1.00	39.24	A	C
ATOM	1188	CG	GLU	A	960	13.184	38.980	22.141	1.00	46.55	A	C
ATOM	1189	CD	GLU	A	960	12.187	40.140	22.010	1.00	48.81	A	C
ATOM	1190	OE1	GLU	A	960	12.358	41.143	22.752	1.00	49.24	A	O
ATOM	1191	OE2	GLU	A	960	11.244	40.048	21.183	1.00	46.66	A	O
ATOM	1192	C	GLU	A	960	13.252	36.721	19.002	1.00	35.00	A	C
ATOM	1193	O	GLU	A	960	14.272	36.044	18.834	1.00	34.68	A	O
ATOM	1194	N	ALA	A	961	12.060	36.361	18.547	1.00	32.61	A	N
ATOM	1195	CA	ALA	A	961	11.884	35.114	17.825	1.00	31.46	A	C
ATOM	1196	CB	ALA	A	961	10.787	34.309	18.475	1.00	33.09	A	C
ATOM	1197	C	ALA	A	961	11.568	35.285	16.349	1.00	29.88	A	C
ATOM	1198	O	ALA	A	961	10.867	34.457	15.787	1.00	30.47	A	O
ATOM	1199	N	HIS	A	962	12.079	36.332	15.709	1.00	27.98	A	N
ATOM	1200	CA	HIS	A	962	11.781	36.552	14.293	1.00	26.94	A	C
ATOM	1201	CB	HIS	A	962	10.367	37.137	14.150	1.00	26.76	A	C
ATOM	1202	CG	HIS	A	962	9.845	37.164	12.746	1.00	29.25	A	C
ATOM	1203	CD2	HIS	A	962	10.482	37.125	11.548	1.00	30.41	A	C
ATOM	1204	ND1	HIS	A	962	8.499	37.259	12.461	1.00	29.15	A	N
ATOM	1205	CE1	HIS	A	962	8.328	37.277	11.149	1.00	29.36	A	C
ATOM	1206	NE2	HIS	A	962	9.515	37.197	10.573	1.00	29.28	A	N
ATOM	1207	C	HIS	A	962	12.785	37.483	13.635	1.00	25.52	A	C
ATOM	1208	O	HIS	A	962	12.830	38.671	13.934	1.00	24.49	A	O
ATOM	1209	N	VAL	A	963	13.583	36.942	12.723	1.00	24.67	A	N
ATOM	1210	CA	VAL	A	963	14.579	37.739	12.020	1.00	22.77	A	C
ATOM	1211	CB	VAL	A	963	15.997	37.135	12.211	1.00	21.51	A	C
ATOM	1212	CG1	VAL	A	963	16.385	37.214	13.677	1.00	18.57	A	C
ATOM	1213	CG2	VAL	A	963	16.043	35.690	11.716	1.00	15.30	A	C
ATOM	1214	C	VAL	A	963	14.253	37.831	10.532	1.00	24.24	A	C
ATOM	1215	O	VAL	A	963	13.710	36.888	9.950	1.00	24.35	A	O
ATOM	1216	N	LYS	A	964	14.577	38.968	9.920	1.00	24.66	A	N
ATOM	1217	CA	LYS	A	964	14.306	39.159	8.493	1.00	26.34	A	C
ATOM	1218	CB	LYS	A	964	13.298	40.291	8.284	1.00	29.10	A	C
ATOM	1219	CG	LYS	A	964	11.887	40.014	8.784	1.00	27.26	A	C
ATOM	1220	CD	LYS	A	964	10.995	41.233	8.537	1.00	26.26	A	C
ATOM	1221	CE	LYS	A	964	9.534	40.902	8.778	1.00	26.90	A	C
ATOM	1222	NZ	LYS	A	964	8.647	42.060	8.526	1.00	30.62	A	N
ATOM	1223	C	LYS	A	964	15.546	39.468	7.665	1.00	25.93	A	C
ATOM	1224	O	LYS	A	964	16.495	40.076	8.155	1.00	28.44	A	O
ATOM	1225	N	ILE	A	965	15.535	39.040	6.408	1.00	24.00	A	N

TABLE 2-continued

ATOM	1226	CA	ILE	A	965	16.654	39.305	5.510	1.00	23.02	A	C
ATOM	1227	CB	ILE	A	965	16.684	38.296	4.332	1.00	23.20	A	C
ATOM	1228	CG2	ILE	A	965	17.821	38.625	3.385	1.00	21.71	A	C
ATOM	1229	CG1	ILE	A	965	16.894	36.871	4.857	1.00	22.96	A	C
ATOM	1230	CD1	ILE	A	965	16.961	35.812	3.758	1.00	21.77	A	C
ATOM	1231	C	ILE	A	965	16.506	40.735	4.972	1.00	23.73	A	C
ATOM	1232	O	ILE	A	965	15.398	41.173	4.614	1.00	22.06	A	O
ATOM	1233	N	ALA	A	966	17.625	41.460	4.919	1.00	23.15	A	N
ATOM	1234	CA	ALA	A	966	17.627	42.852	4.470	1.00	21.44	A	C
ATOM	1235	CB	ALA	A	966	17.822	43.780	5.676	1.00	19.27	A	C
ATOM	1236	C	ALA	A	966	18.669	43.176	3.410	1.00	21.34	A	C
ATOM	1237	O	ALA	A	966	19.700	42.518	3.319	1.00	19.18	A	O
ATOM	1238	N	ASP	A	967	18.373	44.197	2.605	1.00	20.95	A	N
ATOM	1239	CA	ASP	A	967	19.280	44.669	1.565	1.00	21.84	A	C
ATOM	1240	CB	ASP	A	967	20.620	45.061	2.203	1.00	25.14	A	C
ATOM	1241	CG	ASP	A	967	20.589	46.450	2.832	1.00	28.31	A	C
ATOM	1242	OD1	ASP	A	967	19.687	46.736	3.661	1.00	33.06	A	O
ATOM	1243	OD2	ASP	A	967	21.474	47.260	2.491	1.00	28.34	A	O
ATOM	1244	C	ASP	A	967	19.508	43.681	0.431	1.00	20.89	A	C
ATOM	1245	O	ASP	A	967	20.583	43.615	−0.144	1.00	19.01	A	O
ATOM	1246	N	PHE	A	968	18.472	42.936	0.087	1.00	23.31	A	N
ATOM	1247	CA	PHE	A	968	18.578	41.948	−0.973	1.00	23.74	A	C
ATOM	1248	CB	PHE	A	968	17.660	40.776	−0.643	1.00	22.73	A	C
ATOM	1249	CG	PHE	A	968	16.220	41.174	−0.452	1.00	21.43	A	C
ATOM	1250	CD1	PHE	A	968	15.337	41.180	−1.518	1.00	21.04	A	C
ATOM	1251	CD2	PHE	A	968	15.752	41.535	0.795	1.00	21.28	A	C
ATOM	1252	CE1	PHE	A	968	14.014	41.535	−1.340	1.00	21.80	A	C
ATOM	1253	CE2	PHE	A	968	14.427	41.893	0.977	1.00	21.96	A	C
ATOM	1254	CZ	PHE	A	968	13.558	41.890	−0.094	1.00	21.99	A	C
ATOM	1255	C	PHE	A	968	18.246	42.484	−2.364	1.00	25.69	A	C
ATOM	1256	O	PHE	A	968	17.488	43.454	−2.513	1.00	24.40	A	O
ATOM	1257	N	GLY	A	969	18.841	41.835	−3.368	1.00	27.11	A	N
ATOM	1258	CA	GLY	A	969	18.623	42.164	−4.770	1.00	28.84	A	C
ATOM	1259	C	GLY	A	969	18.930	43.573	−5.239	1.00	28.12	A	C
ATOM	1260	O	GLY	A	969	18.100	44.195	−5.887	1.00	29.45	A	O
ATOM	1261	N	LEU	A	970	20.128	44.066	−4.945	1.00	27.97	A	N
ATOM	1262	CA	LEU	A	970	20.522	45.415	−5.345	1.00	27.04	A	C
ATOM	1263	CB	LEU	A	970	20.882	46.223	−4.098	1.00	27.31	A	C
ATOM	1264	CG	LEU	A	970	19.885	47.280	−3.650	1.00	29.99	A	C
ATOM	1265	CD1	LEU	A	970	18.475	46.876	−4.035	1.00	29.45	A	C
ATOM	1266	CD2	LEU	A	970	20.017	47.474	−2.149	1.00	31.52	A	C
ATOM	1267	C	LEU	A	970	21.705	45.418	−6.313	1.00	25.60	A	C
ATOM	1268	O	LEU	A	970	22.214	46.480	−6.671	1.00	24.22	A	O
ATOM	1269	N	ALA	A	971	22.134	44.234	−6.736	1.00	24.75	A	N
ATOM	1270	CA	ALA	A	971	23.278	44.103	−7.638	1.00	27.57	A	C
ATOM	1271	CB	ALA	A	971	23.325	42.695	−8.231	1.00	26.59	A	C
ATOM	1272	C	ALA	A	971	23.271	45.135	−8.753	1.00	29.20	A	C
ATOM	1273	O	ALA	A	971	24.162	45.980	−8.820	1.00	31.64	A	O
ATOM	1274	N	LYS	A	972	22.259	45.065	−9.615	1.00	29.46	A	N
ATOM	1275	CA	LYS	A	972	22.112	45.979	−10.744	1.00	30.77	A	C
ATOM	1276	CB	LYS	A	972	20.697	45.850	−11.322	1.00	32.32	A	C
ATOM	1277	CG	LYS	A	972	20.347	44.427	−11.749	1.00	34.37	A	C
ATOM	1278	CD	LYS	A	972	21.454	43.844	−12.607	1.00	36.13	A	C
ATOM	1279	CE	LYS	A	972	21.197	42.389	−12.946	1.00	39.38	A	C
ATOM	1280	NZ	LYS	A	972	22.346	41.812	−13.722	1.00	41.41	A	N
ATOM	1281	C	LYS	A	972	22.406	47.446	−10.414	1.00	30.81	A	C
ATOM	1282	O	LYS	A	972	23.055	48.155	−11.182	1.00	30.44	A	O
ATOM	1283	N	LEU	A	973	21.930	47.899	−9.265	1.00	30.52	A	N
ATOM	1284	CA	LEU	A	973	22.141	49.276	−8.858	1.00	29.45	A	C
ATOM	1285	CB	LEU	A	973	21.110	49.654	−7.792	1.00	27.35	A	C
ATOM	1286	CG	LEU	A	973	19.690	50.011	−8.250	1.00	26.99	A	C
ATOM	1287	CD1	LEU	A	973	19.474	49.507	−9.674	1.00	27.84	A	C
ATOM	1288	CD2	LEU	A	973	18.645	49.444	−7.269	1.00	23.63	A	C
ATOM	1289	C	LEU	A	973	23.548	49.544	−8.322	1.00	30.66	A	C
ATOM	1290	O	LEU	A	973	23.988	50.685	−8.308	1.00	30.62	A	O
ATOM	1291	N	LEU	A	974	24.258	48.504	−7.888	1.00	32.78	A	N
ATOM	1292	CA	LEU	A	974	25.589	48.690	−7.314	1.00	35.10	A	C
ATOM	1293	CB	LEU	A	974	26.035	47.429	−6.560	1.00	34.09	A	C
ATOM	1294	CG	LEU	A	974	25.141	47.021	−5.372	1.00	31.33	A	C
ATOM	1295	CD1	LEU	A	974	25.844	46.011	−4.476	1.00	31.22	A	C
ATOM	1296	CD2	LEU	A	974	24.786	48.258	−4.582	1.00	29.58	A	C
ATOM	1297	C	LEU	A	974	26.644	49.095	−8.327	1.00	39.13	A	C
ATOM	1298	O	LEU	A	974	26.683	48.588	−9.444	1.00	39.72	A	O
ATOM	1299	N	PRO	A	975	27.533	50.013	−7.931	1.00	42.43	A	N
ATOM	1300	CD	PRO	A	975	27.809	50.379	−6.532	1.00	41.80	A	C
ATOM	1301	CA	PRO	A	975	28.594	50.500	−8.811	1.00	43.55	A	C
ATOM	1302	CB	PRO	A	975	29.427	51.381	−7.883	1.00	43.38	A	C
ATOM	1303	CG	PRO	A	975	29.288	50.685	−6.574	1.00	42.77	A	C
ATOM	1304	C	PRO	A	975	29.407	49.380	−9.438	1.00	44.80	A	C
ATOM	1305	O	PRO	A	975	29.676	48.370	−8.799	1.00	45.65	A	O

TABLE 2-continued

ATOM	1306	N	LEU	A	976	29.778	49.563	−10.700	1.00	46.34	A	N
ATOM	1307	CA	LEU	A	976	30.580	48.578	−11.403	1.00	47.22	A	C
ATOM	1308	CB	LEU	A	976	30.980	49.108	−12.787	1.00	47.95	A	C
ATOM	1309	CG	LEU	A	976	29.859	49.044	−13.840	1.00	48.59	A	C
ATOM	1310	CD1	LEU	A	976	29.441	47.571	−14.033	1.00	48.06	A	C
ATOM	1311	CD2	LEU	A	976	28.666	49.890	−13.389	1.00	47.77	A	C
ATOM	1312	C	LEU	A	976	31.815	48.314	−10.558	1.00	48.24	A	C
ATOM	1313	O	LEU	A	976	31.776	47.482	−9.643	1.00	49.05	A	O
ATOM	1314	N	ASP	A	977	32.898	49.039	−10.854	1.00	48.80	A	N
ATOM	1315	CA	ASP	A	977	34.163	48.909	−10.119	1.00	48.49	A	C
ATOM	1316	CB	ASP	A	977	35.294	49.712	−10.785	1.00	50.18	A	C
ATOM	1317	CG	ASP	A	977	36.480	49.982	−9.818	1.00	52.34	A	C
ATOM	1318	OD1	ASP	A	977	37.652	49.670	−10.196	1.00	52.04	A	O
ATOM	1319	OD2	ASP	A	977	36.233	50.509	−8.690	1.00	51.47	A	O
ATOM	1320	C	ASP	A	977	34.033	49.427	−8.706	1.00	47.71	A	C
ATOM	1321	O	ASP	A	977	33.806	50.620	−8.506	1.00	47.53	A	O
ATOM	1322	N	LYS	A	978	34.207	48.547	−7.726	1.00	46.64	A	N
ATOM	1323	CA	LYS	A	978	34.139	48.946	−6.315	1.00	46.31	A	C
ATOM	1324	CB	LYS	A	978	33.282	47.950	−5.522	1.00	44.80	A	C
ATOM	1325	CG	LYS	A	978	33.214	48.272	−4.029	1.00	43.21	A	C
ATOM	1326	CD	LYS	A	978	32.755	49.717	−3.804	1.00	41.49	A	C
ATOM	1327	CE	LYS	A	978	32.597	50.038	−2.322	1.00	40.48	A	C
ATOM	1328	NZ	LYS	A	978	31.726	49.077	−1.599	1.00	37.88	A	N
ATOM	1329	C	LYS	A	978	35.552	49.007	−5.714	1.00	46.70	A	C
ATOM	1330	O	LYS	A	978	36.359	48.077	−5.894	1.00	46.71	A	O
ATOM	1331	N	ASP	A	979	35.861	50.097	−5.016	1.00	47.20	A	N
ATOM	1332	CA	ASP	A	979	37.182	50.241	−4.396	1.00	47.47	A	C
ATOM	1333	CB	ASP	A	979	37.659	51.698	−4.492	1.00	49.44	A	C
ATOM	1334	CG	ASP	A	979	39.165	51.840	−4.312	1.00	49.88	A	C
ATOM	1335	OD1	ASP	A	979	39.708	52.886	−4.737	1.00	50.87	A	O
ATOM	1336	OD2	ASP	A	979	39.798	50.921	−3.742	1.00	49.55	A	O
ATOM	1337	C	ASP	A	979	37.052	49.805	−2.942	1.00	45.95	A	C
ATOM	1338	O	ASP	A	979	36.785	50.618	−2.052	1.00	44.33	A	O
ATOM	1339	N	TYR	A	980	37.233	48.505	−2.727	1.00	45.35	A	N
ATOM	1340	CA	TYR	A	980	37.107	47.891	−1.407	1.00	45.75	A	C
ATOM	1341	CB	TYR	A	980	37.086	46.367	−1.557	1.00	42.56	A	C
ATOM	1342	CG	TYR	A	980	35.856	45.844	−2.267	1.00	40.45	A	C
ATOM	1343	CD1	TYR	A	980	34.639	45.743	−1.613	1.00	37.80	A	C
ATOM	1344	CE1	TYR	A	980	33.512	45.271	−2.267	1.00	36.59	A	C
ATOM	1345	CD2	TYR	A	980	35.912	45.461	−3.597	1.00	39.77	A	C
ATOM	1346	CE2	TYR	A	980	34.793	44.993	−4.256	1.00	37.65	A	C
ATOM	1347	CZ	TYR	A	980	33.597	44.898	−3.591	1.00	36.99	A	C
ATOM	1348	OH	TYR	A	980	32.489	44.433	−4.267	1.00	36.66	A	O
ATOM	1349	C	TYR	A	980	38.153	48.296	−0.367	1.00	47.00	A	C
ATOM	1350	O	TYR	A	980	38.011	47.982	0.814	1.00	47.86	A	O
ATOM	1351	N	TYR	A	981	39.196	48.994	−0.800	1.00	48.44	A	N
ATOM	1352	CA	TYR	A	981	40.239	49.433	0.117	1.00	49.65	A	C
ATOM	1353	CB	TYR	A	981	41.552	49.597	−0.641	1.00	51.45	A	C
ATOM	1354	CG	TYR	A	981	42.026	48.307	−1.261	1.00	54.63	A	C
ATOM	1355	CD1	TYR	A	981	42.798	48.311	−2.416	1.00	55.85	A	C
ATOM	1356	CE1	TYR	A	981	43.214	47.127	−3.002	1.00	57.90	A	C
ATOM	1357	CD2	TYR	A	981	41.680	47.080	−0.703	1.00	56.41	A	C
ATOM	1358	CE2	TYR	A	981	42.089	45.888	−1.281	1.00	57.59	A	C
ATOM	1359	CZ	TYR	A	981	42.854	45.919	−2.431	1.00	58.54	A	C
ATOM	1360	OH	TYR	A	981	43.256	44.741	−3.016	1.00	60.20	A	O
ATOM	1361	C	TYR	A	981	39.824	50.743	0.781	1.00	48.81	A	C
ATOM	1362	O	TYR	A	981	40.504	51.260	1.673	1.00	48.86	A	O
ATOM	1363	N	VAL	A	982	38.688	51.266	0.339	1.00	48.42	A	N
ATOM	1364	CA	VAL	A	982	38.140	52.501	0.880	1.00	46.99	A	C
ATOM	1365	CB	VAL	A	982	37.831	53.528	−0.243	1.00	46.43	A	C
ATOM	1366	CG1	VAL	A	982	37.265	54.802	0.359	1.00	45.87	A	C
ATOM	1367	CG2	VAL	A	982	39.090	53.827	−1.045	1.00	44.80	A	C
ATOM	1368	C	VAL	A	982	36.845	52.148	1.605	1.00	46.90	A	C
ATOM	1369	O	VAL	A	982	35.773	52.122	1.004	1.00	45.78	A	O
ATOM	1370	N	VAL	A	983	36.965	51.866	2.898	1.00	47.59	A	N
ATOM	1371	CA	VAL	A	983	35.824	51.510	3.729	1.00	48.25	A	C
ATOM	1372	CB	VAL	A	983	35.733	49.970	3.898	1.00	48.58	A	C
ATOM	1373	CG1	VAL	A	983	37.076	49.417	4.360	1.00	49.17	A	C
ATOM	1374	CG2	VAL	A	983	34.631	49.608	4.884	1.00	47.78	A	C
ATOM	1375	C	VAL	A	983	35.928	52.175	5.100	1.00	49.02	A	C
ATOM	1376	O	VAL	A	983	37.005	52.243	5.691	1.00	49.70	A	O
ATOM	1377	N	ARG	A	984	34.803	52.671	5.601	1.00	49.82	A	N
ATOM	1378	CA	ARG	A	984	34.778	53.333	6.895	1.00	49.53	A	C
ATOM	1379	CB	ARG	A	984	33.426	54.011	7.127	1.00	52.18	A	C
ATOM	1380	CG	ARG	A	984	33.463	55.085	8.205	1.00	55.52	A	C
ATOM	1381	CD	ARG	A	984	32.063	55.466	8.673	1.00	59.59	A	C
ATOM	1382	NE	ARG	A	984	32.062	56.701	9.457	1.00	62.13	A	N
ATOM	1383	CZ	ARG	A	984	32.749	56.885	10.581	1.00	63.45	A	C
ATOM	1384	NH1	ARG	A	984	32.678	58.052	11.210	1.00	64.01	A	N
ATOM	1385	NH2	ARG	A	984	33.499	55.908	11.079	1.00	61.84	A	N

TABLE 2-continued

ATOM	1386	C	ARG	A	984	35.036	52.324	8.001	1.00	48.55	A	C
ATOM	1387	O	ARG	A	984	35.748	52.619	8.962	1.00	49.22	A	O
ATOM	1388	N	GLU	A	985	34.449	51.137	7.871	1.00	46.54	A	N
ATOM	1389	CA	GLU	A	985	34.631	50.081	8.864	1.00	44.17	A	C
ATOM	1390	CB	GLU	A	985	33.338	49.854	9.653	1.00	45.48	A	C
ATOM	1391	CG	GLU	A	985	33.574	49.373	11.092	1.00	50.99	A	C
ATOM	1392	CD	GLU	A	985	33.937	50.504	12.068	1.00	53.46	A	C
ATOM	1393	OE1	GLU	A	985	34.598	50.216	13.094	1.00	54.69	A	O
ATOM	1394	OE2	GLU	A	985	33.549	51.672	11.820	1.00	54.79	A	O
ATOM	1395	C	GLU	A	985	35.050	48.793	8.159	1.00	41.59	A	C
ATOM	1396	O	GLU	A	985	34.220	47.947	7.842	1.00	41.99	A	O
ATOM	1397	N	PRO	A	986	36.363	48.626	7.928	1.00	39.68	A	N
ATOM	1398	CD	PRO	A	986	37.384	49.483	8.550	1.00	37.11	A	C
ATOM	1399	CA	PRO	A	986	36.988	47.476	7.261	1.00	37.84	A	C
ATOM	1400	CB	PRO	A	986	38.479	47.779	7.389	1.00	37.70	A	C
ATOM	1401	CG	PRO	A	986	38.550	48.546	8.663	1.00	37.19	A	C
ATOM	1402	C	PRO	A	986	36.613	46.090	7.788	1.00	36.77	A	C
ATOM	1403	O	PRO	A	986	36.536	45.131	7.026	1.00	37.02	A	O
ATOM	1404	N	GLY	A	987	36.380	45.970	9.085	1.00	35.59	A	N
ATOM	1405	CA	GLY	A	987	36.010	44.671	9.607	1.00	33.97	A	C
ATOM	1406	C	GLY	A	987	34.746	44.114	8.963	1.00	32.82	A	C
ATOM	1407	O	GLY	A	987	34.510	42.912	9.012	1.00	32.56	A	O
ATOM	1408	N	GLN	A	988	33.927	44.974	8.366	1.00	30.14	A	N
ATOM	1409	CA	GLN	A	988	32.700	44.512	7.737	1.00	29.16	A	C
ATOM	1410	CB	GLN	A	988	31.493	45.292	8.268	1.00	30.41	A	C
ATOM	1411	CG	GLN	A	988	31.206	45.078	9.756	1.00	29.44	A	C
ATOM	1412	CD	GLN	A	988	30.776	43.654	10.082	1.00	31.42	A	C
ATOM	1413	OE1	GLN	A	988	29.653	43.244	9.684	1.00	26.26	A	O
ATOM	1414	NE2	GLN	A	988	31.576	42.947	10.735	1.00	32.03	A	O
ATOM	1415	C	GLN	A	988	32.765	44.645	6.226	1.00	29.17	A	C
ATOM	1416	O	GLN	A	988	31.740	44.806	5.570	1.00	27.90	A	O
ATOM	1417	N	SER	A	989	33.978	44.584	5.678	1.00	29.64	A	N
ATOM	1418	CA	SER	A	989	34.172	44.687	4.236	1.00	27.96	A	C
ATOM	1419	CB	SER	A	989	35.656	44.774	3.888	1.00	29.01	A	C
ATOM	1420	OG	SER	A	989	35.843	44.762	2.483	1.00	28.27	A	O
ATOM	1421	C	SER	A	989	33.587	43.442	3.604	1.00	28.16	A	C
ATOM	1422	O	SER	A	989	33.928	42.327	3.982	1.00	26.58	A	O
ATOM	1423	N	PRO	A	990	32.714	43.624	2.608	1.00	28.39	A	N
ATOM	1424	CD	PRO	A	990	32.449	44.935	1.982	1.00	29.19	A	C
ATOM	1425	CA	PRO	A	990	32.035	42.551	1.879	1.00	28.46	A	C
ATOM	1426	CB	PRO	A	990	31.472	43.272	0.653	1.00	29.64	A	C
ATOM	1427	CG	PRO	A	990	31.205	44.662	1.169	1.00	28.86	A	C
ATOM	1428	C	PRO	A	990	32.893	41.355	1.489	1.00	26.71	A	C
ATOM	1429	O	PRO	A	990	32.386	40.242	1.408	1.00	27.68	A	O
ATOM	1430	N	ILE	A	991	34.181	41.590	1.247	1.00	25.64	A	N
ATOM	1431	CA	ILE	A	991	35.109	40.542	0.829	1.00	23.27	A	C
ATOM	1432	CB	ILE	A	991	36.508	41.121	0.543	1.00	22.53	A	C
ATOM	1433	CG2	ILE	A	991	36.390	42.242	−0.472	1.00	21.72	A	C
ATOM	1434	CG1	ILE	A	991	37.162	41.592	1.851	1.00	21.38	A	C
ATOM	1435	CD1	ILE	A	991	38.659	41.885	1.740	1.00	17.35	A	C
ATOM	1436	C	ILE	A	991	35.282	39.340	1.759	1.00	22.89	A	C
ATOM	1437	O	ILE	A	991	35.628	38.267	1.292	1.00	22.75	A	O
ATOM	1438	N	PHE	A	992	35.061	39.504	3.060	1.00	22.83	A	N
ATOM	1439	CA	PHE	A	992	35.218	38.367	3.972	1.00	24.27	A	C
ATOM	1440	CB	PHE	A	992	35.468	38.832	5.423	1.00	21.98	A	C
ATOM	1441	CG	PHE	A	992	36.692	39.675	5.575	1.00	18.63	A	C
ATOM	1442	CD1	PHE	A	992	37.905	39.225	5.092	1.00	19.36	A	C
ATOM	1443	CD2	PHE	A	992	36.621	40.944	6.129	1.00	18.42	A	C
ATOM	1444	CE1	PHE	A	992	39.042	40.021	5.144	1.00	18.38	A	C
ATOM	1445	CE2	PHE	A	992	37.747	41.751	6.188	1.00	20.39	A	C
ATOM	1446	CZ	PHE	A	992	38.965	41.286	5.689	1.00	19.03	A	C
ATOM	1447	C	PHE	A	992	34.010	37.434	3.945	1.00	24.41	A	C
ATOM	1448	O	PHE	A	992	33.986	36.436	4.669	1.00	23.48	A	O
ATOM	1449	N	TRP	A	993	33.014	37.767	3.122	1.00	24.17	A	N
ATOM	1450	CA	TRP	A	993	31.801	36.952	2.977	1.00	24.08	A	C
ATOM	1451	CB	TRP	A	993	30.549	37.762	3.318	1.00	20.25	A	C
ATOM	1452	CG	TRP	A	993	30.322	37.968	4.776	1.00	18.22	A	C
ATOM	1453	CD2	TRP	A	993	30.934	38.962	5.609	1.00	17.81	A	C
ATOM	1454	CE2	TRP	A	993	30.465	38.750	6.923	1.00	16.65	A	C
ATOM	1455	CE3	TRP	A	993	31.836	40.012	5.371	1.00	17.27	A	C
ATOM	1456	CD1	TRP	A	993	29.524	37.222	5.593	1.00	18.48	A	C
ATOM	1457	NE1	TRP	A	993	29.608	37.683	6.885	1.00	18.25	A	N
ATOM	1458	CZ2	TRP	A	993	30.867	39.544	7.998	1.00	16.84	A	C
ATOM	1459	CZ3	TRP	A	993	32.235	40.800	6.439	1.00	13.99	A	C
ATOM	1460	CH2	TRP	A	993	31.752	40.562	7.738	1.00	15.16	A	C
ATOM	1461	C	TRP	A	993	31.674	36.458	1.547	1.00	25.04	A	C
ATOM	1462	O	TRP	A	993	30.772	35.691	1.224	1.00	27.65	A	O
ATOM	1463	N	TYR	A	994	32.590	36.891	0.691	1.00	26.08	A	N
ATOM	1464	CA	TYR	A	994	32.539	36.516	−0.713	1.00	26.22	A	C
ATOM	1465	CB	TYR	A	994	33.385	37.473	−1.556	1.00	26.01	A	C

TABLE 2-continued

ATOM	1466	CG	TYR	A	994	32.752	38.812	−1.830	1.00	25.79	A	C
ATOM	1467	CD1	TYR	A	994	31.565	39.180	−1.224	1.00	25.47	A	C
ATOM	1468	CE1	TYR	A	994	30.997	40.421	−1.472	1.00	29.26	A	C
ATOM	1469	CD2	TYR	A	994	33.358	39.719	−2.695	1.00	27.78	A	C
ATOM	1470	CE2	TYR	A	994	32.798	40.958	−2.949	1.00	27.26	A	C
ATOM	1471	CZ	TYR	A	994	31.620	41.304	−2.337	1.00	28.81	A	C
ATOM	1472	OH	TYR	A	994	31.056	42.529	−2.598	1.00	31.86	A	O
ATOM	1473	C	TYR	A	994	33.018	35.111	−0.989	1.00	26.70	A	C
ATOM	1474	O	TYR	A	994	33.871	34.587	−0.281	1.00	26.37	A	O
ATOM	1475	N	ALA	A	995	32.462	34.516	−2.040	1.00	27.56	A	N
ATOM	1476	CA	ALA	A	995	32.846	33.180	−2.479	1.00	27.85	A	C
ATOM	1477	CB	ALA	A	995	31.653	32.478	−3.148	1.00	26.19	A	C
ATOM	1478	C	ALA	A	995	33.980	33.383	−3.488	1.00	28.75	A	C
ATOM	1479	O	ALA	A	995	34.156	34.486	−4.027	1.00	29.61	A	O
ATOM	1480	N	PRO	A	996	34.762	32.329	−3.760	1.00	27.48	A	N
ATOM	1481	CD	PRO	A	996	34.696	30.981	−3.181	1.00	26.63	A	C
ATOM	1482	CA	PRO	A	996	35.872	32.429	−4.711	1.00	28.77	A	C
ATOM	1483	CB	PRO	A	996	36.309	30.978	−4.880	1.00	26.97	A	C
ATOM	1484	CG	PRO	A	996	36.050	30.418	−3.535	1.00	25.72	A	C
ATOM	1485	C	PRO	A	996	35.494	33.082	−6.041	1.00	29.95	A	C
ATOM	1486	O	PRO	A	996	36.092	34.089	−6.423	1.00	32.04	A	O
ATOM	1487	N	GLU	A	997	34.507	32.517	−6.736	1.00	30.01	A	N
ATOM	1488	CA	GLU	A	997	34.080	33.050	−8.026	1.00	30.26	A	C
ATOM	1489	CB	GLU	A	997	32.822	32.323	−8.549	1.00	30.28	A	C
ATOM	1490	CG	GLU	A	997	31.606	32.373	−7.648	1.00	30.56	A	C
ATOM	1491	CD	GLU	A	997	31.601	31.268	−6.606	1.00	32.94	A	C
ATOM	1492	OE1	GLU	A	997	32.683	30.961	−6.052	1.00	31.09	A	O
ATOM	1493	OE2	GLU	A	997	30.506	30.717	−6.338	1.00	33.32	A	O
ATOM	1494	C	GLU	A	997	33.829	34.550	−7.948	1.00	30.85	A	C
ATOM	1495	O	GLU	A	997	34.057	35.281	−8.909	1.00	31.80	A	O
ATOM	1496	N	SER	A	998	33.368	35.017	−6.797	1.00	32.03	A	N
ATOM	1497	CA	SER	A	998	33.132	36.440	−6.626	1.00	32.09	A	C
ATOM	1498	CB	SER	A	998	32.300	36.688	−5.379	1.00	31.27	A	C
ATOM	1499	OG	SER	A	998	30.955	36.327	−5.607	1.00	32.96	A	O
ATOM	1500	C	SER	A	998	34.442	37.214	−6.522	1.00	32.18	A	C
ATOM	1501	O	SER	A	998	34.644	38.198	−7.224	1.00	34.53	A	O
ATOM	1502	N	LEU	A	999	35.329	36.770	−5.642	1.00	32.83	A	N
ATOM	1503	CA	LEU	A	999	36.606	37.447	−5.448	1.00	33.92	A	C
ATOM	1504	CB	LEU	A	999	37.435	36.730	−4.374	1.00	31.31	A	C
ATOM	1505	CG	LEU	A	999	37.076	36.949	−2.897	1.00	29.60	A	C
ATOM	1506	CD1	LEU	A	999	37.992	36.101	−2.035	1.00	28.05	A	C
ATOM	1507	CD2	LEU	A	999	37.226	38.417	−2.515	1.00	28.42	A	C
ATOM	1508	C	LEU	A	999	37.432	37.568	−6.724	1.00	35.90	A	C
ATOM	1509	O	LEU	A	999	38.101	38.574	−6.936	1.00	36.64	A	O
ATOM	1510	N	SER	A	1000	37.374	36.556	−7.581	1.00	36.91	A	N
ATOM	1511	CA	SER	A	1000	38.152	36.566	−8.808	1.00	37.30	A	C
ATOM	1512	CB	SER	A	1000	38.755	35.192	−9.032	1.00	36.47	A	C
ATOM	1513	OG	SER	A	1000	37.724	34.247	−9.246	1.00	34.60	A	O
ATOM	1514	C	SER	A	1000	37.425	36.977	−10.084	1.00	39.08	A	C
ATOM	1515	O	SER	A	1000	38.062	37.421	−11.033	1.00	40.17	A	O
ATOM	1516	N	ASP	A	1001	36.109	36.831	−10.132	1.00	40.32	A	N
ATOM	1517	CA	ASP	A	1001	35.396	37.191	−11.351	1.00	42.54	A	C
ATOM	1518	CB	ASP	A	1001	35.041	35.925	−12.126	1.00	43.98	A	C
ATOM	1519	CG	ASP	A	1001	36.266	35.162	−12.574	1.00	45.00	A	C
ATOM	1520	OD1	ASP	A	1001	37.062	35.734	−13.349	1.00	44.52	A	O
ATOM	1521	OD2	ASP	A	1001	36.433	33.998	−12.147	1.00	45.98	A	O
ATOM	1522	C	ASP	A	1001	34.142	38.031	−11.171	1.00	42.36	A	C
ATOM	1523	O	ASP	A	1001	33.359	38.178	−12.104	1.00	42.53	A	O
ATOM	1524	N	ASN	A	1002	33.957	38.589	−9.983	1.00	42.42	A	N
ATOM	1525	CA	ASN	A	1002	32.781	39.390	−9.703	1.00	42.92	A	C
ATOM	1526	CB	ASN	A	1002	32.703	40.590	−10.641	1.00	44.00	A	C
ATOM	1527	CG	ASN	A	1002	33.246	41.847	−10.015	1.00	45.61	A	C
ATOM	1528	OD1	ASN	A	1002	34.455	42.005	−9.846	1.00	49.08	A	O
ATOM	1529	ND2	ASN	A	1002	32.349	42.753	−9.653	1.00	45.40	A	N
ATOM	1530	C	ASN	A	1002	31.514	38.570	−9.841	1.00	42.00	A	C
ATOM	1531	O	ASN	A	1002	30.421	39.095	−9.676	1.00	43.55	A	O
ATOM	1532	N	ILE	A	1003	31.667	37.285	−10.143	1.00	40.07	A	N
ATOM	1533	CA	ILE	A	1003	30.535	36.376	−10.303	1.00	37.80	A	C
ATOM	1534	CB	ILE	A	1003	30.994	34.944	−10.651	1.00	38.03	A	C
ATOM	1535	CG2	ILE	A	1003	29.822	33.987	−10.536	1.00	35.71	A	C
ATOM	1536	CG1	ILE	A	1003	31.629	34.902	−12.037	1.00	35.29	A	C
ATOM	1537	CD1	ILE	A	1003	31.993	33.514	−12.454	1.00	33.06	A	C
ATOM	1538	C	ILE	A	1003	29.704	36.255	−9.037	1.00	37.43	A	C
ATOM	1539	O	ILE	A	1003	30.230	35.936	−7.969	1.00	38.59	A	O
ATOM	1540	N	PHE	A	1004	28.404	36.488	−9.170	1.00	36.18	A	N
ATOM	1541	CA	PHE	A	1004	27.474	36.390	−8.055	1.00	34.51	A	C
ATOM	1542	CB	PHE	A	1004	27.055	37.787	−7.598	1.00	32.45	A	C
ATOM	1543	CG	PHE	A	1004	28.126	38.525	−6.828	1.00	34.32	A	C
ATOM	1544	CD1	PHE	A	1004	28.492	38.110	−5.549	1.00	32.69	A	C
ATOM	1545	CD2	PHE	A	1004	28.757	39.637	−7.371	1.00	31.98	A	C

TABLE 2-continued

ATOM	1546	CE1	PHE	A	1004	29.462	38.789	−4.824	1.00	31.46	A	C
ATOM	1547	CE2	PHE	A	1004	29.730	40.322	−6.651	1.00	33.05	A	C
ATOM	1548	CZ	PHE	A	1004	30.081	39.895	−5.373	1.00	32.10	A	C
ATOM	1549	C	PHE	A	1004	26.256	35.591	−8.511	1.00	35.47	A	C
ATOM	1550	O	PHE	A	1004	25.696	35.854	−9.575	1.00	37.28	A	O
ATOM	1551	N	SER	A	1005	25.853	34.610	−7.709	1.00	34.92	A	N
ATOM	1552	CA	SER	A	1005	24.713	33.774	−8.045	1.00	32.73	A	C
ATOM	1553	CB	SER	A	1005	25.158	32.584	−8.888	1.00	33.36	A	C
ATOM	1554	OG	SER	A	1005	25.959	31.704	−8.114	1.00	36.71	A	O
ATOM	1555	C	SER	A	1005	24.051	33.245	−6.794	1.00	31.68	A	C
ATOM	1556	O	SER	A	1005	24.536	33.449	−5.681	1.00	31.32	A	O
ATOM	1557	N	ARG	A	1006	22.937	32.553	−6.996	1.00	29.32	A	N
ATOM	1558	CA	ARG	A	1006	22.197	31.961	−5.900	1.00	28.94	A	C
ATOM	1559	CB	ARG	A	1006	21.040	31.130	−6.452	1.00	29.85	A	C
ATOM	1560	CG	ARG	A	1006	20.005	31.949	−7.202	1.00	35.55	A	C
ATOM	1561	CD	ARG	A	1006	18.924	31.062	−7.843	1.00	38.40	A	C
ATOM	1562	NE	ARG	A	1006	18.345	30.128	−6.876	1.00	43.57	A	N
ATOM	1563	CZ	ARG	A	1006	17.471	29.168	−7.174	1.00	44.56	A	C
ATOM	1564	NH1	ARG	A	1006	17.009	28.367	−6.220	1.00	41.70	A	N
ATOM	1565	NH2	ARG	A	1006	17.053	29.012	−8.420	1.00	44.91	A	N
ATOM	1566	C	ARG	A	1006	23.125	31.068	−5.081	1.00	27.76	A	C
ATOM	1567	O	ARG	A	1006	22.995	30.967	−3.861	1.00	25.65	A	O
ATOM	1568	N	GLN	A	1007	24.077	30.433	−5.755	1.00	27.21	A	N
ATOM	1569	CA	GLN	A	1007	24.979	29.524	−5.067	1.00	27.69	A	C
ATOM	1570	CB	GLN	A	1007	25.552	28.492	−6.041	1.00	27.27	A	C
ATOM	1571	CG	GLN	A	1007	24.566	27.386	−6.456	1.00	30.11	A	C
ATOM	1572	CD	GLN	A	1007	24.008	26.541	−5.273	1.00	32.03	A	C
ATOM	1573	OE1	GLN	A	1007	22.897	26.788	−4.771	1.00	28.18	A	O
ATOM	1574	NE2	GLN	A	1007	24.785	25.542	−4.836	1.00	29.04	A	N
ATOM	1575	C	GLN	A	1007	26.093	30.236	−4.313	1.00	27.70	A	C
ATOM	1576	O	GLN	A	1007	26.567	29.750	−3.276	1.00	26.19	A	O
ATOM	1577	N	SER	A	1008	26.506	31.390	−4.822	1.00	26.86	A	N
ATOM	1578	CA	SER	A	1008	27.542	32.155	−4.150	1.00	26.66	A	C
ATOM	1579	CB	SER	A	1008	27.997	33.331	−5.018	1.00	29.18	A	C
ATOM	1580	OG	SER	A	1008	26.903	34.144	−5.400	1.00	31.80	A	O
ATOM	1581	C	SER	A	1008	26.950	32.654	−2.830	1.00	26.32	A	C
ATOM	1582	O	SER	A	1008	27.659	32.816	−1.828	1.00	26.69	A	O
ATOM	1583	N	ASP	A	1009	25.641	32.892	−2.830	1.00	25.13	A	N
ATOM	1584	CA	ASP	A	1009	24.974	33.341	−1.620	1.00	24.62	A	C
ATOM	1585	CB	ASP	A	1009	23.493	33.663	−1.882	1.00	26.26	A	C
ATOM	1586	CG	ASP	A	1009	23.275	35.087	−2.421	1.00	29.77	A	C
ATOM	1587	OD1	ASP	A	1009	22.195	35.364	−2.993	1.00	31.03	A	O
ATOM	1588	OD2	ASP	A	1009	24.175	35.937	−2.268	1.00	30.20	A	O
ATOM	1589	C	ASP	A	1009	25.097	32.221	−0.602	1.00	23.09	A	C
ATOM	1590	O	ASP	A	1009	25.382	32.469	0.566	1.00	24.34	A	O
ATOM	1591	N	VAL	A	1010	24.904	30.987	−1.051	1.00	21.87	A	N
ATOM	1592	CA	VAL	A	1010	24.986	29.833	−0.155	1.00	21.43	A	C
ATOM	1593	CB	VAL	A	1010	24.906	28.497	−0.933	1.00	18.75	A	C
ATOM	1594	CG1	VAL	A	1010	25.308	27.344	−0.033	1.00	18.01	A	C
ATOM	1595	CG2	VAL	A	1010	23.499	28.277	−1.432	1.00	17.23	A	C
ATOM	1596	C	VAL	A	1010	26.279	29.868	0.649	1.00	21.21	A	C
ATOM	1597	O	VAL	A	1010	26.285	29.538	1.827	1.00	18.67	A	O
ATOM	1598	N	TRP	A	1011	27.355	30.289	−0.012	1.00	22.19	A	N
ATOM	1599	CA	TRP	A	1011	28.671	30.408	0.582	1.00	21.30	A	C
ATOM	1600	CB	TRP	A	1011	29.676	30.823	−0.494	1.00	21.09	A	C
ATOM	1601	CG	TRP	A	1011	31.004	31.272	0.051	1.00	22.20	A	C
ATOM	1602	CD2	TRP	A	1011	32.242	30.555	−0.013	1.00	23.32	A	C
ATOM	1603	CE2	TRP	A	1011	33.216	31.343	0.643	1.00	23.77	A	C
ATOM	1604	CE3	TRP	A	1011	32.622	29.326	−0.558	1.00	23.63	A	C
ATOM	1605	CD1	TRP	A	1011	31.271	32.436	0.726	1.00	22.11	A	C
ATOM	1606	NE1	TRP	A	1011	32.596	32.484	1.084	1.00	22.41	A	N
ATOM	1607	CZ2	TRP	A	1011	34.546	30.940	0.769	1.00	23.00	A	C
ATOM	1608	CZ3	TRP	A	1011	33.949	28.926	−0.433	1.00	25.04	A	C
ATOM	1609	CH2	TRP	A	1011	34.893	29.734	0.226	1.00	24.41	A	C
ATOM	1610	C	TRP	A	1011	28.642	31.456	1.690	1.00	21.41	A	C
ATOM	1611	O	TRP	A	1011	29.159	31.231	2.780	1.00	20.92	A	O
ATOM	1612	N	SER	A	1012	28.035	32.602	1.401	1.00	22.30	A	N
ATOM	1613	CA	SER	A	1012	27.940	33.684	2.373	1.00	21.76	A	C
ATOM	1614	CB	SER	A	1012	27.286	34.926	1.742	1.00	24.85	A	C
ATOM	1615	OG	SER	A	1012	27.933	35.297	0.534	1.00	28.52	A	O
ATOM	1616	C	SER	A	1012	27.107	33.232	3.565	1.00	19.93	A	C
ATOM	1617	O	SER	A	1012	27.303	33.713	4.677	1.00	20.35	A	O
ATOM	1618	N	PHE	A	1013	26.167	32.322	3.332	1.00	18.72	A	N
ATOM	1619	CA	PHE	A	1013	25.324	31.823	4.409	1.00	19.74	A	C
ATOM	1620	CB	PHE	A	1013	24.197	30.958	3.850	1.00	21.64	A	C
ATOM	1621	CG	PHE	A	1013	23.267	30.431	4.902	1.00	21.29	A	C
ATOM	1622	CD1	PHE	A	1013	22.582	31.307	5.738	1.00	21.35	A	C
ATOM	1623	CD2	PHE	A	1013	23.048	29.069	5.033	1.00	20.51	A	C
ATOM	1624	CE1	PHE	A	1013	21.689	30.832	6.684	1.00	20.93	A	C
ATOM	1625	CE2	PHE	A	1013	22.156	28.579	5.973	1.00	21.44	A	C

TABLE 2-continued

ATOM	1626	CZ	PHE	A	1013	21.470	29.462	6.804	1.00	21.79	A	C
ATOM	1627	C	PHE	A	1013	26.191	31.002	5.355	1.00	18.87	A	C
ATOM	1628	O	PHE	A	1013	25.924	30.912	6.549	1.00	18.16	A	O
ATOM	1629	N	GLY	A	1014	27.236	30.399	4.806	1.00	19.32	A	N
ATOM	1630	CA	GLY	A	1014	28.143	29.634	5.639	1.00	23.18	A	C
ATOM	1631	C	GLY	A	1014	28.825	30.545	6.654	1.00	24.21	A	C
ATOM	1632	O	GLY	A	1014	28.994	30.177	7.815	1.00	23.51	A	O
ATOM	1633	N	VAL	A	1015	29.206	31.745	6.216	1.00	25.95	A	N
ATOM	1634	CA	VAL	A	1015	29.874	32.705	7.093	1.00	26.43	A	C
ATOM	1635	CB	VAL	A	1015	30.547	33.841	6.282	1.00	25.36	A	C
ATOM	1636	CG1	VAL	A	1015	31.399	34.710	7.195	1.00	26.40	A	C
ATOM	1637	CG2	VAL	A	1015	31.404	33.253	5.185	1.00	24.13	A	C
ATOM	1638	C	VAL	A	1015	28.873	33.305	8.070	1.00	27.70	A	C
ATOM	1639	O	VAL	A	1015	29.229	33.721	9.174	1.00	29.33	A	O
ATOM	1640	N	VAL	A	1016	27.610	33.345	7.674	1.00	26.63	A	N
ATOM	1641	CA	VAL	A	1016	26.600	33.897	8.559	1.00	26.58	A	C
ATOM	1642	CB	VAL	A	1016	25.275	34.134	7.813	1.00	27.70	A	C
ATOM	1643	CG1	VAL	A	1016	24.194	34.545	8.804	1.00	25.02	A	C
ATOM	1644	CG2	VAL	A	1016	25.469	35.196	6.738	1.00	24.95	A	C
ATOM	1645	C	VAL	A	1016	26.363	32.924	9.709	1.00	26.56	A	C
ATOM	1646	O	VAL	A	1016	26.105	33.334	10.843	1.00	25.68	A	O
ATOM	1647	N	LEU	A	1017	26.445	31.630	9.406	1.00	25.79	A	N
ATOM	1648	CA	LEU	A	1017	26.259	30.595	10.420	1.00	25.37	A	C
ATOM	1649	CB	LEU	A	1017	26.231	29.204	9.768	1.00	24.57	A	C
ATOM	1650	CG	LEU	A	1017	24.935	28.765	9.069	1.00	23.17	A	C
ATOM	1651	CD1	LEU	A	1017	25.212	27.540	8.190	1.00	22.94	A	C
ATOM	1652	CD2	LEU	A	1017	23.856	28.468	10.107	1.00	19.40	A	C
ATOM	1653	C	LEU	A	1017	27.417	30.702	11.404	1.00	25.14	A	C
ATOM	1654	O	LEU	A	1017	27.242	30.556	12.609	1.00	24.28	A	O
ATOM	1655	N	TYR	A	1018	28.603	30.964	10.871	1.00	26.09	A	N
ATOM	1656	CA	TYR	A	1018	29.788	31.130	11.687	1.00	27.05	A	C
ATOM	1657	CB	TYR	A	1018	31.003	31.388	10.801	1.00	28.96	A	C
ATOM	1658	CG	TYR	A	1018	32.276	31.654	11.584	1.00	32.69	A	C
ATOM	1659	CD1	TYR	A	1018	32.924	30.627	12.263	1.00	31.98	A	C
ATOM	1660	CE1	TYR	A	1018	34.082	30.865	12.978	1.00	31.92	A	C
ATOM	1661	CD2	TYR	A	1018	32.830	32.936	11.647	1.00	31.48	A	C
ATOM	1662	CE2	TYR	A	1018	33.993	33.180	12.364	1.00	31.23	A	C
ATOM	1663	CZ	TYR	A	1018	34.610	32.139	13.023	1.00	32.76	A	C
ATOM	1664	OH	TYR	A	1018	35.763	32.357	13.732	1.00	34.73	A	O
ATOM	1665	C	TYR	A	1018	29.590	32.316	12.636	1.00	28.41	A	C
ATOM	1666	O	TYR	A	1018	29.937	32.228	13.807	1.00	29.27	A	O
ATOM	1667	N	GLU	A	1019	29.024	33.416	12.130	1.00	28.77	A	N
ATOM	1668	CA	GLU	A	1019	28.786	34.623	12.931	1.00	28.13	A	C
ATOM	1669	CB	GLU	A	1019	28.258	35.773	12.046	1.00	29.97	A	C
ATOM	1670	CG	GLU	A	1019	29.188	36.251	10.919	1.00	29.60	A	C
ATOM	1671	CD	GLU	A	1019	28.738	37.577	10.299	1.00	29.59	A	C
ATOM	1672	OE1	GLU	A	1019	28.910	38.638	10.937	1.00	31.77	A	O
ATOM	1673	OE2	GLU	A	1019	28.208	37.564	9.171	1.00	28.17	A	O
ATOM	1674	C	GLU	A	1019	27.796	34.396	14.086	1.00	27.33	A	C
ATOM	1675	O	GLU	A	1019	27.988	34.897	15.195	1.00	25.68	A	O
ATOM	1676	N	LEU	A	1020	26.730	33.650	13.825	1.00	27.14	A	N
ATOM	1677	CA	LEU	A	1020	25.735	33.394	14.855	1.00	26.16	A	C
ATOM	1678	CB	LEU	A	1020	24.513	32.683	14.255	1.00	25.72	A	C
ATOM	1679	CG	LEU	A	1020	23.673	33.449	13.223	1.00	27.06	A	C
ATOM	1680	CD1	LEU	A	1020	22.199	33.148	13.464	1.00	26.70	A	C
ATOM	1681	CD2	LEU	A	1020	23.917	34.949	13.329	1.00	26.86	A	C
ATOM	1682	C	LEU	A	1020	26.318	32.560	15.988	1.00	25.00	A	C
ATOM	1683	O	LEU	A	1020	26.214	32.929	17.153	1.00	23.85	A	O
ATOM	1684	N	PHE	A	1021	26.935	31.438	15.637	1.00	25.96	A	N
ATOM	1685	CA	PHE	A	1021	27.540	30.551	16.622	1.00	28.26	A	C
ATOM	1686	CB	PHE	A	1021	27.756	29.173	15.998	1.00	28.65	A	C
ATOM	1687	CG	PHE	A	1021	26.514	28.328	15.974	1.00	30.48	A	C
ATOM	1688	CD1	PHE	A	1021	26.105	27.648	17.107	1.00	30.22	A	C
ATOM	1689	CD2	PHE	A	1021	25.721	28.270	14.846	1.00	31.61	A	C
ATOM	1690	CE1	PHE	A	1021	24.932	26.932	17.119	1.00	32.06	A	C
ATOM	1691	CE2	PHE	A	1021	24.537	27.552	14.853	1.00	33.64	A	C
ATOM	1692	CZ	PHE	A	1021	24.145	26.882	15.994	1.00	33.78	A	C
ATOM	1693	C	PHE	A	1021	28.848	31.115	17.184	1.00	29.12	A	C
ATOM	1694	O	PHE	A	1021	29.517	30.477	17.992	1.00	30.42	A	O
ATOM	1695	N	THR	A	1022	29.190	32.325	16.751	1.00	29.23	A	N
ATOM	1696	CA	THR	A	1022	30.386	33.014	17.201	1.00	28.15	A	C
ATOM	1697	CB	THR	A	1022	31.291	33.380	15.994	1.00	28.82	A	C
ATOM	1698	OG1	THR	A	1022	32.643	32.998	16.273	1.00	30.39	A	O
ATOM	1699	CG2	THR	A	1022	31.237	34.859	15.693	1.00	28.63	A	C
ATOM	1700	C	THR	A	1022	29.899	34.276	17.905	1.00	28.32	A	C
ATOM	1701	O	THR	A	1022	30.692	35.071	18.422	1.00	27.51	A	O
ATOM	1702	N	TYR	A	1023	28.573	34.427	17.931	1.00	28.68	A	N
ATOM	1703	CA	TYR	A	1023	27.897	35.573	18.545	1.00	27.59	A	C
ATOM	1704	CB	TYR	A	1023	28.003	35.531	20.067	1.00	27.08	A	C
ATOM	1705	CG	TYR	A	1023	27.151	34.471	20.710	1.00	27.19	A	C

TABLE 2-continued

ATOM	1706	CD1	TYR	A	1023	27.691	33.252	21.089	1.00	27.11	A	C
ATOM	1707	CE1	TYR	A	1023	26.900	32.281	21.682	1.00	26.29	A	C
ATOM	1708	CD2	TYR	A	1023	25.799	34.690	20.937	1.00	26.09	A	C
ATOM	1709	CE2	TYR	A	1023	25.006	33.730	21.524	1.00	25.32	A	C
ATOM	1710	CZ	TYR	A	1023	25.559	32.528	21.896	1.00	26.71	A	C
ATOM	1711	OH	TYR	A	1023	24.766	31.569	22.484	1.00	27.13	A	O
ATOM	1712	C	TYR	A	1023	28.471	36.886	18.062	1.00	26.01	A	C
ATOM	1713	O	TYR	A	1023	28.307	37.913	18.712	1.00	26.91	A	O
ATOM	1714	N	CYS	A	1024	29.150	36.849	16.924	1.00	24.48	A	N
ATOM	1715	CA	CYS	A	1024	29.760	38.042	16.359	1.00	27.84	A	C
ATOM	1716	CB	CYS	A	1024	28.698	39.077	15.971	1.00	27.22	A	C
ATOM	1717	SG	CYS	A	1024	27.882	38.643	14.441	1.00	31.28	A	S
ATOM	1718	C	CYS	A	1024	30.787	38.681	17.266	1.00	28.38	A	C
ATOM	1719	O	CYS	A	1024	30.903	39.905	17.346	1.00	28.99	A	O
ATOM	1720	N	ASP	A	1025	31.543	37.845	17.950	1.00	28.57	A	N
ATOM	1721	CA	ASP	A	1025	32.582	38.353	18.807	1.00	30.59	A	C
ATOM	1722	CB	ASP	A	1025	33.163	37.211	19.630	1.00	35.06	A	C
ATOM	1723	CG	ASP	A	1025	34.099	37.697	20.698	1.00	39.47	A	C
ATOM	1724	OD1	ASP	A	1025	33.658	38.530	21.525	1.00	42.23	A	O
ATOM	1725	OD2	ASP	A	1025	35.269	37.249	20.704	1.00	42.12	A	O
ATOM	1726	C	ASP	A	1025	33.647	38.945	17.874	1.00	30.39	A	C
ATOM	1727	O	ASP	A	1025	34.007	38.326	16.870	1.00	29.56	A	O
ATOM	1728	N	LYS	A	1026	34.139	40.136	18.201	1.00	31.27	A	N
ATOM	1729	CA	LYS	A	1026	35.143	40.817	17.381	1.00	33.10	A	C
ATOM	1730	CB	LYS	A	1026	35.401	42.228	17.914	1.00	35.51	A	C
ATOM	1731	CG	LYS	A	1026	34.153	43.016	18.261	1.00	39.16	A	C
ATOM	1732	CD	LYS	A	1026	33.229	43.169	17.082	1.00	42.21	A	C
ATOM	1733	CE	LYS	A	1026	33.853	43.995	15.984	1.00	43.30	A	C
ATOM	1734	NZ	LYS	A	1026	32.833	44.288	14.939	1.00	46.56	A	N
ATOM	1735	C	LYS	A	1026	36.468	40.065	17.327	1.00	33.00	A	C
ATOM	1736	O	LYS	A	1026	37.176	40.116	16.323	1.00	32.10	A	O
ATOM	1737	N	SER	A	1027	36.797	39.368	18.410	1.00	34.41	A	N
ATOM	1738	CA	SER	A	1027	38.042	38.605	18.491	1.00	34.79	A	C
ATOM	1739	CB	SER	A	1027	38.153	37.909	19.856	1.00	33.89	A	C
ATOM	1740	OG	SER	A	1027	37.889	38.809	20.914	1.00	38.74	A	O
ATOM	1741	C	SER	A	1027	38.156	37.545	17.391	1.00	34.36	A	C
ATOM	1742	O	SER	A	1027	39.198	37.413	16.750	1.00	33.83	A	O
ATOM	1743	N	CYS	A	1028	37.080	36.790	17.178	1.00	33.80	A	N
ATOM	1744	CA	CYS	A	1028	37.075	35.716	16.182	1.00	32.68	A	C
ATOM	1745	CB	CYS	A	1028	36.650	34.408	16.850	1.00	32.82	A	C
ATOM	1746	SG	CYS	A	1028	35.060	34.533	17.704	1.00	33.09	A	S
ATOM	1747	C	CYS	A	1028	36.164	35.973	14.982	1.00	30.73	A	C
ATOM	1748	O	CYS	A	1028	35.772	35.043	14.282	1.00	30.74	A	O
ATOM	1749	N	SER	A	1029	35.827	37.230	14.741	1.00	29.90	A	N
ATOM	1750	CA	SER	A	1029	34.959	37.558	13.626	1.00	29.19	A	C
ATOM	1751	CB	SER	A	1029	34.726	39.067	13.567	1.00	28.86	A	C
ATOM	1752	OG	SER	A	1029	35.884	39.732	13.096	1.00	31.25	A	O
ATOM	1753	C	SER	A	1029	35.598	37.086	12.327	1.00	28.26	A	C
ATOM	1754	O	SER	A	1029	36.762	36.669	12.303	1.00	30.05	A	O
ATOM	1755	N	PRO	A	1030	34.834	37.121	11.229	1.00	25.74	A	N
ATOM	1756	CD	PRO	A	1030	33.369	37.260	11.198	1.00	22.85	A	C
ATOM	1757	CA	PRO	A	1030	35.350	36.694	9.928	1.00	24.51	A	C
ATOM	1758	CB	PRO	A	1030	34.149	36.904	9.017	1.00	23.05	A	C
ATOM	1759	CG	PRO	A	1030	33.010	36.539	9.929	1.00	24.45	A	C
ATOM	1760	C	PRO	A	1030	36.605	37.469	9.475	1.00	24.86	A	C
ATOM	1761	O	PRO	A	1030	37.535	36.898	8.872	1.00	23.18	A	O
ATOM	1762	N	SER	A	1031	36.632	38.766	9.768	1.00	24.48	A	N
ATOM	1763	CA	SER	A	1031	37.772	39.609	9.406	1.00	24.82	A	C
ATOM	1764	CB	SER	A	1031	37.422	41.084	9.609	1.00	21.99	A	C
ATOM	1765	OG	SER	A	1031	36.210	41.207	10.327	1.00	27.23	A	O
ATOM	1766	C	SER	A	1031	39.013	39.245	10.231	1.00	25.14	A	C
ATOM	1767	O	SER	A	1031	40.072	38.938	9.685	1.00	25.36	A	O
ATOM	1768	N	ALA	A	1032	38.875	39.279	11.548	1.00	27.52	A	N
ATOM	1769	CA	ALA	A	1032	39.979	38.950	12.435	1.00	28.18	A	C
ATOM	1770	CB	ALA	A	1032	39.474	38.857	13.876	1.00	27.52	A	C
ATOM	1771	C	ALA	A	1032	40.668	37.648	12.031	1.00	29.01	A	C
ATOM	1772	O	ALA	A	1032	41.877	37.637	11.783	1.00	30.30	A	O
ATOM	1773	N	GLU	A	1033	39.905	36.556	11.966	1.00	29.03	A	N
ATOM	1774	CA	GLU	A	1033	40.458	35.247	11.593	1.00	28.45	A	C
ATOM	1775	CB	GLU	A	1033	39.354	34.183	11.531	1.00	31.07	A	C
ATOM	1776	CG	GLU	A	1033	38.745	33.851	12.870	1.00	33.50	A	C
ATOM	1777	CD	GLU	A	1033	39.798	33.685	13.925	1.00	35.91	A	C
ATOM	1778	OE1	GLU	A	1033	40.810	33.015	13.637	1.00	37.80	A	O
ATOM	1779	OE2	GLU	A	1033	39.615	34.220	15.036	1.00	36.97	A	O
ATOM	1780	C	GLU	A	1033	41.190	35.262	10.260	1.00	26.35	A	C
ATOM	1781	O	GLU	A	1033	42.372	34.948	10.186	1.00	25.54	A	O
ATOM	1782	N	PHE	A	1034	40.479	35.610	9.199	1.00	27.44	A	N
ATOM	1783	CA	PHE	A	1034	41.083	35.649	7.879	1.00	27.26	A	C
ATOM	1784	CB	PHE	A	1034	40.080	36.198	6.872	1.00	26.93	A	C
ATOM	1785	CG	PHE	A	1034	39.129	35.165	6.337	1.00	29.70	A	C

TABLE 2-continued

ATOM	1786	CD1	PHE	A	1034	37.809	35.493	6.063	1.00	29.12	A	C
ATOM	1787	CD2	PHE	A	1034	39.566	33.882	6.055	1.00	28.02	A	C
ATOM	1788	CE1	PHE	A	1034	36.947	34.559	5.517	1.00	29.46	A	C
ATOM	1789	CE2	PHE	A	1034	38.707	32.950	5.508	1.00	29.09	A	C
ATOM	1790	CZ	PHE	A	1034	37.396	33.289	5.238	1.00	29.30	A	C
ATOM	1791	C	PHE	A	1034	42.323	36.512	7.899	1.00	27.70	A	C
ATOM	1792	O	PHE	A	1034	43.342	36.168	7.298	1.00	28.43	A	O
ATOM	1793	N	LEU	A	1035	42.242	37.635	8.600	1.00	28.83	A	N
ATOM	1794	CA	LEU	A	1035	43.371	38.550	8.668	1.00	31.32	A	C
ATOM	1795	CB	LEU	A	1035	42.936	39.863	9.326	1.00	30.92	A	C
ATOM	1796	CG	LEU	A	1035	43.110	41.158	8.527	1.00	29.53	A	C
ATOM	1797	CD1	LEU	A	1035	42.484	41.056	7.144	1.00	27.99	A	C
ATOM	1798	CD2	LEU	A	1035	42.468	42.274	9.318	1.00	29.65	A	C
ATOM	1799	C	LEU	A	1035	44.560	37.936	9.408	1.00	33.17	A	C
ATOM	1800	O	LEU	A	1035	45.703	38.007	8.938	1.00	31.72	A	O
ATOM	1801	N	ARG	A	1036	44.300	37.322	10.560	1.00	31.84	A	N
ATOM	1802	CA	ARG	A	1036	45.395	36.717	11.292	1.00	34.63	A	C
ATOM	1803	CB	ARG	A	1036	45.012	36.432	12.746	1.00	34.04	A	C
ATOM	1804	CG	ARG	A	1036	43.831	35.531	12.933	1.00	36.91	A	C
ATOM	1805	CD	ARG	A	1036	43.730	35.091	14.385	1.00	36.17	A	C
ATOM	1806	NE	ARG	A	1036	44.811	34.176	14.715	1.00	34.71	A	N
ATOM	1807	CZ	ARG	A	1036	44.721	32.855	14.611	1.00	33.73	A	C
ATOM	1808	NH1	ARG	A	1036	43.590	32.298	14.203	1.00	32.21	A	N
ATOM	1809	NH2	ARG	A	1036	45.775	32.093	14.879	1.00	33.32	A	N
ATOM	1810	C	ARG	A	1036	45.890	35.441	10.621	1.00	36.65	A	C
ATOM	1811	O	ARG	A	1036	47.060	35.084	10.752	1.00	38.90	A	O
ATOM	1812	N	MET	A	1037	45.014	34.764	9.886	1.00	38.66	A	N
ATOM	1813	CA	MET	A	1037	45.404	33.539	9.207	1.00	40.19	A	C
ATOM	1814	CB	MET	A	1037	44.189	32.894	8.525	1.00	41.26	A	C
ATOM	1815	CG	MET	A	1037	43.389	31.971	9.443	1.00	41.69	A	C
ATOM	1816	SD	MET	A	1037	41.858	31.301	8.730	1.00	42.48	A	S
ATOM	1817	CE	MET	A	1037	42.498	30.138	7.523	1.00	42.39	A	C
ATOM	1818	C	MET	A	1037	46.516	33.791	8.192	1.00	41.59	A	C
ATOM	1819	O	MET	A	1037	47.477	33.023	8.108	1.00	42.63	A	O
ATOM	1820	N	MET	A	1038	46.398	34.871	7.428	1.00	43.48	A	N
ATOM	1821	CA	MET	A	1038	47.418	35.187	6.433	1.00	43.88	A	C
ATOM	1822	CB	MET	A	1038	46.753	35.624	5.120	1.00	44.08	A	C
ATOM	1823	CG	MET	A	1038	45.450	36.379	5.283	1.00	44.10	A	C
ATOM	1824	SD	MET	A	1038	44.666	36.794	3.686	1.00	42.80	A	S
ATOM	1825	CE	MET	A	1038	43.115	37.477	4.272	1.00	43.10	A	C
ATOM	1826	C	MET	A	1038	48.457	36.218	6.897	1.00	44.50	A	C
ATOM	1827	O	MET	A	1038	49.252	36.722	6.096	1.00	44.74	A	O
ATOM	1828	N	GLY	A	1039	48.443	36.508	8.196	1.00	44.49	A	N
ATOM	1829	CA	GLY	A	1039	49.394	37.434	8.791	1.00	45.60	A	C
ATOM	1830	C	GLY	A	1039	49.386	38.877	8.331	1.00	46.45	A	C
ATOM	1831	O	GLY	A	1039	50.383	39.579	8.503	1.00	46.86	A	O
ATOM	1832	N	CYS	A	1040	48.265	39.324	7.768	1.00	47.04	A	N
ATOM	1833	CA	CYS	A	1040	48.124	40.690	7.270	1.00	45.91	A	C
ATOM	1834	CB	CYS	A	1040	46.874	40.805	6.406	1.00	44.80	A	C
ATOM	1835	SG	CYS	A	1040	46.619	42.464	5.760	1.00	44.01	A	S
ATOM	1836	C	CYS	A	1040	48.033	41.715	8.392	1.00	46.80	A	C
ATOM	1837	O	CYS	A	1040	47.246	41.552	9.321	1.00	45.47	A	O
ATOM	1838	N	GLU	A	1041	48.834	42.774	8.299	1.00	47.51	A	N
ATOM	1839	CA	GLU	A	1041	48.823	43.823	9.314	1.00	49.46	A	C
ATOM	1840	CB	GLU	A	1041	50.229	44.395	9.504	1.00	49.04	A	C
ATOM	1841	CG	GLU	A	1041	51.136	44.225	8.317	1.00	49.42	A	C
ATOM	1842	CD	GLU	A	1041	52.547	44.678	8.612	1.00	50.81	A	C
ATOM	1843	OE1	GLU	A	1041	53.438	44.401	7.784	1.00	50.66	A	O
ATOM	1844	OE2	GLU	A	1041	52.765	45.315	9.670	1.00	50.52	A	O
ATOM	1845	C	GLU	A	1041	47.834	44.929	8.957	1.00	50.58	A	C
ATOM	1846	O	GLU	A	1041	47.369	45.680	9.822	1.00	50.40	A	O
ATOM	1847	N	ARG	A	1042	47.522	45.017	7.668	1.00	50.93	A	N
ATOM	1848	CA	ARG	A	1042	46.558	45.985	7.164	1.00	51.11	A	C
ATOM	1849	CB	ARG	A	1042	46.623	46.047	5.638	1.00	52.02	A	C
ATOM	1850	CG	ARG	A	1042	47.953	46.510	5.094	1.00	54.33	A	C
ATOM	1851	CD	ARG	A	1042	47.964	46.457	3.580	1.00	56.72	A	C
ATOM	1852	NE	ARG	A	1042	48.896	47.432	3.029	1.00	58.81	A	N
ATOM	1853	CZ	ARG	A	1042	48.728	48.746	3.124	1.00	59.85	A	C
ATOM	1854	NH1	ARG	A	1042	47.661	49.232	3.746	1.00	59.79	A	N
ATOM	1855	NH2	ARG	A	1042	49.629	49.572	2.609	1.00	60.58	A	N
ATOM	1856	C	ARG	A	1042	45.177	45.499	7.583	1.00	50.01	A	C
ATOM	1857	O	ARG	A	1042	44.984	44.308	7.843	1.00	49.66	A	O
ATOM	1858	N	ASP	A	1043	44.210	46.406	7.644	1.00	48.38	A	N
ATOM	1859	CA	ASP	A	1043	42.866	46.002	8.031	1.00	46.88	A	C
ATOM	1860	CB	ASP	A	1043	42.072	47.208	8.536	1.00	48.76	A	C
ATOM	1861	CG	ASP	A	1043	42.676	47.815	9.780	1.00	50.44	A	C
ATOM	1862	OD1	ASP	A	1043	43.032	47.040	10.692	1.00	49.73	A	O
ATOM	1863	OD2	ASP	A	1043	42.793	49.061	9.848	1.00	53.87	A	O
ATOM	1864	C	ASP	A	1043	42.131	45.344	6.869	1.00	44.75	A	C
ATOM	1865	O	ASP	A	1043	41.085	44.720	7.058	1.00	44.07	A	O

TABLE 2-continued

ATOM	1866	N	VAL	A	1044	42.686	45.487	5.669	1.00	43.28	A	N
ATOM	1867	CA	VAL	A	1044	42.088	44.918	4.461	1.00	42.27	A	C
ATOM	1868	CB	VAL	A	1044	41.217	45.960	3.700	1.00	39.69	A	C
ATOM	1869	CG1	VAL	A	1044	40.503	45.297	2.552	1.00	38.77	A	C
ATOM	1870	CG2	VAL	A	1044	40.219	46.602	4.631	1.00	39.30	A	C
ATOM	1871	C	VAL	A	1044	43.219	44.479	3.543	1.00	41.86	A	C
ATOM	1872	O	VAL	A	1044	43.960	45.303	3.018	1.00	42.88	A	O
ATOM	1873	N	PRO	A	1045	43.353	43.170	3.328	1.00	41.70	A	N
ATOM	1874	CD	PRO	A	1045	42.500	42.111	3.901	1.00	42.62	A	C
ATOM	1875	CA	PRO	A	1045	44.394	42.596	2.477	1.00	41.48	A	C
ATOM	1876	CB	PRO	A	1045	44.510	41.181	3.013	1.00	42.55	A	C
ATOM	1877	CG	PRO	A	1045	43.055	40.839	3.243	1.00	42.55	A	C
ATOM	1878	C	PRO	A	1045	44.017	42.597	1.007	1.00	41.10	A	C
ATOM	1879	O	PRO	A	1045	42.840	42.654	0.672	1.00	41.90	A	O
ATOM	1880	N	ALA	A	1046	45.018	42.532	0.133	1.00	40.68	A	N
ATOM	1881	CA	ALA	A	1046	44.763	42.478	−1.300	1.00	40.27	A	C
ATOM	1882	CB	ALA	A	1046	46.063	42.224	−2.060	1.00	38.59	A	C
ATOM	1883	C	ALA	A	1046	43.797	41.313	−1.500	1.00	40.14	A	C
ATOM	1884	O	ALA	A	1046	43.802	40.359	−0.718	1.00	39.01	A	O
ATOM	1885	N	LEU	A	1047	42.973	41.387	−2.540	1.00	39.96	A	N
ATOM	1886	CA	LEU	A	1047	42.002	40.330	−2.801	1.00	39.57	A	C
ATOM	1887	CB	LEU	A	1047	40.917	40.840	−3.754	1.00	40.40	A	C
ATOM	1888	CG	LEU	A	1047	39.964	41.889	−3.172	1.00	41.57	A	C
ATOM	1889	CD1	LEU	A	1047	40.729	42.949	−2.374	1.00	41.75	A	C
ATOM	1890	CD2	LEU	A	1047	39.193	42.524	−4.306	1.00	41.77	A	C
ATOM	1891	C	LEU	A	1047	42.651	39.070	−3.364	1.00	39.02	A	C
ATOM	1892	O	LEU	A	1047	42.210	37.954	−3.084	1.00	37.37	A	O
ATOM	1893	N	CYS	A	1048	43.700	39.247	−4.156	1.00	37.99	A	N
ATOM	1894	CA	CYS	A	1048	44.390	38.105	−4.735	1.00	39.05	A	C
ATOM	1895	CB	CYS	A	1048	45.504	38.576	−5.687	1.00	40.67	A	C
ATOM	1896	SG	CYS	A	1048	46.817	39.620	−4.933	1.00	44.56	A	S
ATOM	1897	C	CYS	A	1048	44.974	37.254	−3.609	1.00	38.04	A	C
ATOM	1898	O	CYS	A	1048	45.072	36.038	−3.726	1.00	37.74	A	O
ATOM	1899	N	ARG	A	1049	45.337	37.912	−2.512	1.00	37.48	A	N
ATOM	1900	CA	ARG	A	1049	45.903	37.260	−1.334	1.00	38.07	A	C
ATOM	1901	CB	ARG	A	1049	46.426	38.334	−0.385	1.00	41.00	A	C
ATOM	1902	CG	ARG	A	1049	47.138	37.822	0.848	1.00	44.03	A	C
ATOM	1903	CD	ARG	A	1049	47.472	38.995	1.746	1.00	49.13	A	C
ATOM	1904	NE	ARG	A	1049	48.367	38.655	2.849	1.00	52.70	A	N
ATOM	1905	CZ	ARG	A	1049	48.742	39.529	3.777	1.00	54.00	A	C
ATOM	1906	NH1	ARG	A	1049	49.559	39.168	4.756	1.00	54.29	A	N
ATOM	1907	NH2	ARG	A	1049	48.288	40.775	3.722	1.00	55.55	A	N
ATOM	1908	C	ARG	A	1049	44.845	36.408	−0.616	1.00	36.85	A	C
ATOM	1909	O	ARG	A	1049	45.070	35.237	−0.297	1.00	35.82	A	O
ATOM	1910	N	LEU	A	1050	43.695	37.022	−0.359	1.00	33.99	A	N
ATOM	1911	CA	LEU	A	1050	42.583	36.357	0.296	1.00	33.03	A	C
ATOM	1912	CB	LEU	A	1050	41.436	37.352	0.511	1.00	31.26	A	C
ATOM	1913	CG	LEU	A	1050	40.191	36.791	1.203	1.00	31.23	A	C
ATOM	1914	CD1	LEU	A	1050	40.584	36.118	2.516	1.00	31.70	A	C
ATOM	1915	CD2	LEU	A	1050	39.196	37.891	1.447	1.00	27.72	A	C
ATOM	1916	C	LEU	A	1050	42.110	35.184	−0.564	1.00	32.10	A	C
ATOM	1917	O	LEU	A	1050	41.851	34.098	−0.050	1.00	29.58	A	O
ATOM	1918	N	LEU	A	1051	42.001	35.413	−1.870	1.00	32.63	A	N
ATOM	1919	CA	LEU	A	1051	41.587	34.376	−2.813	1.00	34.32	A	C
ATOM	1920	CB	LEU	A	1051	41.476	34.957	−4.226	1.00	33.80	A	C
ATOM	1921	CG	LEU	A	1051	41.255	33.929	−5.342	1.00	34.32	A	C
ATOM	1922	CD1	LEU	A	1051	39.849	33.357	−5.237	1.00	31.96	A	C
ATOM	1923	CD2	LEU	A	1051	41.469	34.582	−6.716	1.00	33.65	A	C
ATOM	1924	C	LEU	A	1051	42.603	33.233	−2.817	1.00	34.75	A	C
ATOM	1925	O	LEU	A	1051	42.243	32.065	−2.967	1.00	34.98	A	O
ATOM	1926	N	GLU	A	1052	43.875	33.586	−2.663	1.00	35.72	A	N
ATOM	1927	CA	GLU	A	1052	44.958	32.609	−2.631	1.00	36.23	A	C
ATOM	1928	CB	GLU	A	1052	46.304	33.326	−2.548	1.00	39.64	A	C
ATOM	1929	CG	GLU	A	1052	47.475	32.427	−2.167	1.00	43.74	A	C
ATOM	1930	CD	GLU	A	1052	48.809	33.137	−2.295	1.00	46.95	A	C
ATOM	1931	OE1	GLU	A	1052	49.015	34.155	−1.591	1.00	48.67	A	O
ATOM	1932	OE2	GLU	A	1052	49.644	32.678	−3.106	1.00	47.66	A	O
ATOM	1933	C	GLU	A	1052	44.811	31.692	−1.429	1.00	35.08	A	C
ATOM	1934	O	GLU	A	1052	45.019	30.487	−1.522	1.00	33.30	A	O
ATOM	1935	N	LEU	A	1053	44.469	32.281	−0.292	1.00	35.01	A	N
ATOM	1936	CA	LEU	A	1053	44.285	31.518	0.930	1.00	32.96	A	C
ATOM	1937	CB	LEU	A	1053	43.964	32.459	2.096	1.00	30.50	A	C
ATOM	1938	CG	LEU	A	1053	43.745	31.774	3.443	1.00	30.65	A	C
ATOM	1939	CD1	LEU	A	1053	45.030	31.079	3.864	1.00	32.92	A	C
ATOM	1940	CD2	LEU	A	1053	43.321	32.784	4.487	1.00	32.45	A	C
ATOM	1941	C	LEU	A	1053	43.144	30.521	0.743	1.00	32.04	A	C
ATOM	1942	O	LEU	A	1053	43.240	29.378	1.182	1.00	32.79	A	O
ATOM	1943	N	LEU	A	1054	42.072	30.958	0.085	1.00	31.62	A	N
ATOM	1944	CA	LEU	A	1054	40.907	30.105	−0.145	1.00	31.95	A	C
ATOM	1945	CB	LEU	A	1054	39.682	30.957	−0.527	1.00	30.46	A	C

TABLE 2-continued

ATOM	1946	CG	LEU	A	1054	39.007	31.743	0.619	1.00	28.90	A	C
ATOM	1947	CD1	LEU	A	1054	37.990	32.716	0.083	1.00	27.05	A	C
ATOM	1948	CD2	LEU	A	1054	38.336	30.776	1.571	1.00	28.35	A	C
ATOM	1949	C	LEU	A	1054	41.176	29.056	−1.212	1.00	32.04	A	C
ATOM	1950	O	LEU	A	1054	40.636	27.951	−1.152	1.00	30.77	A	O
ATOM	1951	N	GLU	A	1055	42.022	29.406	−2.178	1.00	34.23	A	N
ATOM	1952	CA	GLU	A	1055	42.391	28.499	−3.261	1.00	35.51	A	C
ATOM	1953	CB	GLU	A	1055	43.157	29.265	−4.344	1.00	35.87	A	C
ATOM	1954	CG	GLU	A	1055	42.246	30.077	−5.257	1.00	39.71	A	C
ATOM	1955	CD	GLU	A	1055	42.980	30.842	−6.353	1.00	39.88	A	C
ATOM	1956	OE1	GLU	A	1055	42.318	31.202	−7.349	1.00	39.86	A	O
ATOM	1957	OE2	GLU	A	1055	44.199	31.095	−6.223	1.00	40.73	A	O
ATOM	1958	C	GLU	A	1055	43.228	27.321	−2.764	1.00	36.34	A	C
ATOM	1959	O	GLU	A	1055	43.353	26.306	−3.445	1.00	35.49	A	O
ATOM	1960	N	GLU	A	1056	43.799	27.456	−1.575	1.00	37.58	A	N
ATOM	1961	CA	GLU	A	1056	44.615	26.396	−1.014	1.00	38.62	A	C
ATOM	1962	CB	GLU	A	1056	45.799	26.980	−0.239	1.00	40.75	A	C
ATOM	1963	CG	GLU	A	1056	46.638	27.967	−1.050	1.00	46.03	A	C
ATOM	1964	CD	GLU	A	1056	47.817	28.551	−0.266	1.00	49.39	A	C
ATOM	1965	OE1	GLU	A	1056	47.625	29.026	0.879	1.00	50.27	A	O
ATOM	1966	OE2	GLU	A	1056	48.944	28.544	−0.812	1.00	51.90	A	O
ATOM	1967	C	GLU	A	1056	43.776	25.541	−0.090	1.00	38.57	A	C
ATOM	1968	O	GLU	A	1056	44.303	24.669	0.596	1.00	39.87	A	O
ATOM	1969	N	GLY	A	1057	42.473	25.803	−0.061	1.00	37.04	A	N
ATOM	1970	CA	GLY	A	1057	41.579	25.030	0.784	1.00	36.00	A	C
ATOM	1971	C	GLY	A	1057	41.388	25.534	2.203	1.00	36.34	A	C
ATOM	1972	O	GLY	A	1057	40.717	24.884	3.007	1.00	37.96	A	O
ATOM	1973	N	GLN	A	1058	41.959	26.691	2.520	1.00	34.56	A	N
ATOM	1974	CA	GLN	A	1058	41.837	27.261	3.855	1.00	33.27	A	C
ATOM	1975	CB	GLN	A	1058	42.883	28.358	4.032	1.00	34.13	A	C
ATOM	1976	CG	GLN	A	1058	44.307	27.852	3.907	1.00	35.03	A	C
ATOM	1977	CD	GLN	A	1058	44.927	27.530	5.250	1.00	36.09	A	C
ATOM	1978	OE1	GLN	A	1058	44.310	26.873	6.087	1.00	37.42	A	O
ATOM	1979	NE2	GLN	A	1058	46.159	27.989	5.461	1.00	35.08	A	N
ATOM	1980	C	GLN	A	1058	40.435	27.820	4.122	1.00	33.23	A	C
ATOM	1981	O	GLN	A	1058	39.807	28.399	3.236	1.00	33.08	A	O
ATOM	1982	N	ARG	A	1059	39.951	27.646	5.349	1.00	31.87	A	N
ATOM	1983	CA	ARG	A	1059	38.626	28.123	5.724	1.00	31.24	A	C
ATOM	1984	CB	ARG	A	1059	37.595	26.995	5.609	1.00	28.73	A	C
ATOM	1985	CG	ARG	A	1059	37.471	26.382	4.211	1.00	30.52	A	C
ATOM	1986	CD	ARG	A	1059	36.676	27.284	3.264	1.00	31.00	A	C
ATOM	1987	NE	ARG	A	1059	36.415	26.677	1.960	1.00	27.97	A	N
ATOM	1988	CZ	ARG	A	1059	37.266	26.682	0.936	1.00	27.94	A	C
ATOM	1989	NH1	ARG	A	1059	38.448	27.265	1.046	1.00	24.82	A	N
ATOM	1990	NH2	ARG	A	1059	36.934	26.100	−0.210	1.00	28.85	A	N
ATOM	1991	C	ARG	A	1059	38.664	28.618	7.158	1.00	31.11	A	C
ATOM	1992	O	ARG	A	1059	39.686	28.523	7.817	1.00	31.41	A	O
ATOM	1993	N	LEU	A	1060	37.548	29.162	7.627	1.00	33.19	A	N
ATOM	1994	CA	LEU	A	1060	37.441	29.660	8.987	1.00	34.25	A	C
ATOM	1995	CB	LEU	A	1060	36.165	30.477	9.142	1.00	32.03	A	C
ATOM	1996	CG	LEU	A	1060	36.057	31.822	8.416	1.00	34.02	A	C
ATOM	1997	CD1	LEU	A	1060	34.688	32.454	8.726	1.00	32.53	A	C
ATOM	1998	CD2	LEU	A	1060	37.182	32.749	8.854	1.00	30.27	A	C
ATOM	1999	C	LEU	A	1060	37.413	28.517	9.998	1.00	36.03	A	C
ATOM	2000	O	LEU	A	1060	36.772	27.495	9.769	1.00	36.83	A	O
ATOM	2001	N	PRO	A	1061	38.112	28.678	11.132	1.00	37.96	A	N
ATOM	2002	CD	PRO	A	1061	38.966	29.821	11.495	1.00	37.87	A	C
ATOM	2003	CA	PRO	A	1061	38.153	27.652	12.180	1.00	39.04	A	C
ATOM	2004	CB	PRO	A	1061	39.247	28.154	13.110	1.00	38.27	A	C
ATOM	2005	CG	PRO	A	1061	39.108	29.640	12.998	1.00	38.72	A	C
ATOM	2006	C	PRO	A	1061	36.821	27.544	12.907	1.00	41.03	A	C
ATOM	2007	O	PRO	A	1061	36.318	28.537	13.428	1.00	44.44	A	O
ATOM	2008	N	ALA	A	1062	36.264	26.337	12.943	1.00	41.14	A	N
ATOM	2009	CA	ALA	A	1062	34.997	26.075	13.615	1.00	41.14	A	C
ATOM	2010	CB	ALA	A	1062	34.888	24.596	13.941	1.00	40.50	A	C
ATOM	2011	C	ALA	A	1062	34.867	26.890	14.894	1.00	41.04	A	C
ATOM	2012	O	ALA	A	1062	35.752	26.870	15.744	1.00	42.44	A	O
ATOM	2013	N	PRO	A	1063	33.759	27.627	15.044	1.00	40.13	A	N
ATOM	2014	CD	PRO	A	1063	32.615	27.790	14.130	1.00	37.87	A	C
ATOM	2015	CA	PRO	A	1063	33.586	28.426	16.257	1.00	41.05	A	C
ATOM	2016	CB	PRO	A	1063	32.262	29.153	16.003	1.00	38.84	A	C
ATOM	2017	CG	PRO	A	1063	31.540	28.242	15.057	1.00	38.22	A	C
ATOM	2018	C	PRO	A	1063	33.584	27.547	17.518	1.00	42.11	A	C
ATOM	2019	O	PRO	A	1063	33.066	26.431	17.513	1.00	41.67	A	O
ATOM	2020	N	PRO	A	1064	34.190	28.045	18.607	1.00	43.41	A	N
ATOM	2021	CD	PRO	A	1064	34.900	29.335	18.645	1.00	42.90	A	C
ATOM	2022	CA	PRO	A	1064	34.301	27.363	19.902	1.00	43.90	A	C
ATOM	2023	CB	PRO	A	1064	34.942	28.425	20.794	1.00	42.85	A	C
ATOM	2024	CG	PRO	A	1064	35.826	29.152	19.838	1.00	42.18	A	C
ATOM	2025	C	PRO	A	1064	32.986	26.853	20.475	1.00	44.26	A	C

TABLE 2-continued

ATOM	2026	O	PRO	A	1064	32.100	27.641	20.809	1.00	45.70	A	O
ATOM	2027	N	ALA	A	1065	32.879	25.530	20.589	1.00	43.97	A	N
ATOM	2028	CA	ALA	A	1065	31.699	24.866	21.141	1.00	44.07	A	C
ATOM	2029	CB	ALA	A	1065	31.305	25.523	22.459	1.00	42.97	A	C
ATOM	2030	C	ALA	A	1065	30.508	24.854	20.187	1.00	44.37	A	C
ATOM	2031	O	ALA	A	1065	29.356	24.964	20.611	1.00	45.07	A	O
ATOM	2032	N	CYS	A	1066	30.784	24.706	18.900	1.00	43.46	A	N
ATOM	2033	CA	CYS	A	1066	29.723	24.696	17.909	1.00	43.03	A	C
ATOM	2034	CB	CYS	A	1066	30.255	25.251	16.582	1.00	43.32	A	C
ATOM	2035	SG	CYS	A	1066	28.994	25.547	15.320	1.00	45.07	A	S
ATOM	2036	C	CYS	A	1066	29.188	23.284	17.714	1.00	42.43	A	C
ATOM	2037	O	CYS	A	1066	29.952	22.318	17.665	1.00	42.66	A	O
ATOM	2038	N	PRO	A	1067	27.860	23.144	17.616	1.00	40.86	A	N
ATOM	2039	CD	PRO	A	1067	26.841	24.185	17.802	1.00	40.79	A	C
ATOM	2040	CA	PRO	A	1067	27.236	21.834	17.423	1.00	40.84	A	C
ATOM	2041	CB	PRO	A	1067	25.766	22.185	17.246	1.00	41.20	A	C
ATOM	2042	CG	PRO	A	1067	25.617	23.370	18.152	1.00	40.13	A	C
ATOM	2043	C	PRO	A	1067	27.831	21.147	16.200	1.00	40.94	A	C
ATOM	2044	O	PRO	A	1067	27.826	21.700	15.096	1.00	42.30	A	O
ATOM	2045	N	ALA	A	1068	28.351	19.943	16.409	1.00	39.79	A	N
ATOM	2046	CA	ALA	A	1068	28.977	19.168	15.344	1.00	39.39	A	C
ATOM	2047	CB	ALA	A	1068	29.105	17.706	15.779	1.00	37.82	A	C
ATOM	2048	C	ALA	A	1068	28.261	19.254	13.993	1.00	38.42	A	C
ATOM	2049	O	ALA	A	1068	28.881	19.558	12.970	1.00	36.38	A	O
ATOM	2050	N	GLU	A	1069	26.959	18.985	13.992	1.00	38.56	A	N
ATOM	2051	CA	GLU	A	1069	26.185	19.013	12.761	1.00	40.94	A	C
ATOM	2052	CB	GLU	A	1069	24.825	18.344	12.980	1.00	43.16	A	C
ATOM	2053	CG	GLU	A	1069	24.115	18.787	14.246	1.00	48.31	A	C
ATOM	2054	CD	GLU	A	1069	24.606	18.064	15.490	1.00	48.90	A	C
ATOM	2055	OE1	GLU	A	1069	24.303	16.860	15.636	1.00	48.25	A	O
ATOM	2056	OE2	GLU	A	1069	25.291	18.704	16.318	1.00	50.20	A	O
ATOM	2057	C	GLU	A	1069	26.004	20.416	12.170	1.00	40.52	A	C
ATOM	2058	O	GLU	A	1069	25.711	20.561	10.984	1.00	40.07	A	O
ATOM	2059	N	VAL	A	1070	26.182	21.447	12.990	1.00	39.74	A	N
ATOM	2060	CA	VAL	A	1070	26.056	22.822	12.511	1.00	39.24	A	C
ATOM	2061	CB	VAL	A	1070	25.897	23.811	13.679	1.00	39.84	A	C
ATOM	2062	CG1	VAL	A	1070	26.045	25.229	13.167	1.00	41.40	A	C
ATOM	2063	CG2	VAL	A	1070	24.542	23.633	14.337	1.00	40.18	A	C
ATOM	2064	C	VAL	A	1070	27.307	23.207	11.715	1.00	38.46	A	C
ATOM	2065	O	VAL	A	1070	27.232	23.876	10.683	1.00	35.39	A	O
ATOM	2066	N	HIS	A	1071	28.461	22.774	12.211	1.00	39.05	A	N
ATOM	2067	CA	HIS	A	1071	29.731	23.049	11.561	1.00	38.75	A	C
ATOM	2068	CB	HIS	A	1071	30.880	22.686	12.506	1.00	39.65	A	C
ATOM	2069	CG	HIS	A	1071	32.235	22.962	11.939	1.00	40.75	A	C
ATOM	2070	CD2	HIS	A	1071	33.282	22.138	11.693	1.00	41.51	A	C
ATOM	2071	ND1	HIS	A	1071	32.618	24.212	11.508	1.00	42.40	A	N
ATOM	2072	CE1	HIS	A	1071	33.843	24.147	11.014	1.00	42.63	A	C
ATOM	2073	NE2	HIS	A	1071	34.267	22.900	11.115	1.00	43.15	A	N
ATOM	2074	C	HIS	A	1071	29.847	22.265	10.248	1.00	38.96	A	C
ATOM	2075	O	HIS	A	1071	30.521	22.696	9.308	1.00	38.24	A	O
ATOM	2076	N	GLU	A	1072	29.176	21.119	10.172	1.00	38.32	A	N
ATOM	2077	CA	GLU	A	1072	29.233	20.318	8.955	1.00	39.59	A	C
ATOM	2078	CB	GLU	A	1072	28.687	18.914	9.213	1.00	44.08	A	C
ATOM	2079	CG	GLU	A	1072	29.130	17.901	8.180	1.00	49.99	A	C
ATOM	2080	CD	GLU	A	1072	29.125	16.493	8.735	1.00	55.49	A	C
ATOM	2081	OE1	GLU	A	1072	28.020	15.960	8.998	1.00	57.05	A	O
ATOM	2082	OE2	GLU	A	1072	30.231	15.930	8.919	1.00	57.75	A	O
ATOM	2083	C	GLU	A	1072	28.458	20.975	7.814	1.00	37.22	A	C
ATOM	2084	O	GLU	A	1072	28.882	20.927	6.657	1.00	36.12	A	O
ATOM	2085	N	LEU	A	1073	27.324	21.586	8.146	1.00	34.76	A	N
ATOM	2086	CA	LEU	A	1073	26.502	22.270	7.156	1.00	34.30	A	C
ATOM	2087	CB	LEU	A	1073	25.197	22.783	7.793	1.00	33.32	A	C
ATOM	2088	CG	LEU	A	1073	24.188	21.723	8.263	1.00	32.92	A	C
ATOM	2089	CD1	LEU	A	1073	22.954	22.376	8.870	1.00	32.52	A	C
ATOM	2090	CD2	LEU	A	1073	23.802	20.851	7.070	1.00	32.45	A	C
ATOM	2091	C	LEU	A	1073	27.281	23.444	6.567	1.00	34.69	A	C
ATOM	2092	O	LEU	A	1073	27.421	23.569	5.347	1.00	34.74	A	O
ATOM	2093	N	MET	A	1074	27.806	24.298	7.437	1.00	34.59	A	N
ATOM	2094	CA	MET	A	1074	28.549	25.441	6.961	1.00	33.88	A	C
ATOM	2095	CB	MET	A	1074	28.911	26.381	8.113	1.00	33.70	A	C
ATOM	2096	CG	MET	A	1074	30.006	25.915	9.028	1.00	32.46	A	C
ATOM	2097	SD	MET	A	1074	30.443	27.221	10.202	1.00	30.20	A	S
ATOM	2098	CE	MET	A	1074	28.953	27.318	11.178	1.00	24.80	A	C
ATOM	2099	C	MET	A	1074	29.790	24.960	6.245	1.00	34.28	A	C
ATOM	2100	O	MET	A	1074	30.260	25.598	5.309	1.00	36.55	A	O
ATOM	2101	N	LYS	A	1075	30.313	23.818	6.672	1.00	33.90	A	N
ATOM	2102	CA	LYS	A	1075	31.498	23.258	6.034	1.00	33.51	A	C
ATOM	2103	CB	LYS	A	1075	31.914	21.970	6.742	1.00	35.85	A	C
ATOM	2104	CG	LYS	A	1075	33.385	21.659	6.671	1.00	35.71	A	C
ATOM	2105	CD	LYS	A	1075	34.094	22.141	7.929	1.00	37.92	A	C

TABLE 2-continued

ATOM	2106	CE	LYS	A	1075	35.611	22.142	7.732	1.00	39.92	A	C
ATOM	2107	NZ	LYS	A	1075	36.041	23.064	6.618	1.00	37.97	A	N
ATOM	2108	C	LYS	A	1075	31.150	22.954	4.572	1.00	32.67	A	C
ATOM	2109	O	LYS	A	1075	31.969	23.147	3.688	1.00	34.17	A	O
ATOM	2110	N	LEU	A	1076	29.926	22.476	4.340	1.00	30.61	A	N
ATOM	2111	CA	LEU	A	1076	29.419	22.154	3.004	1.00	28.22	A	C
ATOM	2112	CB	LEU	A	1076	28.101	21.389	3.127	1.00	27.15	A	C
ATOM	2113	CG	LEU	A	1076	28.083	20.006	3.787	1.00	27.60	A	C
ATOM	2114	CD1	LEU	A	1076	26.637	19.545	3.999	1.00	25.25	A	C
ATOM	2115	CD2	LEU	A	1076	28.831	19.031	2.911	1.00	24.89	A	C
ATOM	2116	C	LEU	A	1076	29.175	23.409	2.147	1.00	28.61	A	C
ATOM	2117	O	LEU	A	1076	29.316	23.383	0.923	1.00	27.41	A	O
ATOM	2118	N	CYS	A	1077	28.785	24.502	2.796	1.00	26.68	A	N
ATOM	2119	CA	CYS	A	1077	28.529	25.746	2.088	1.00	24.29	A	C
ATOM	2120	CB	CYS	A	1077	27.953	26.794	3.032	1.00	21.98	A	C
ATOM	2121	SG	CYS	A	1077	26.297	26.455	3.616	1.00	19.81	A	S
ATOM	2122	C	CYS	A	1077	29.798	26.301	1.476	1.00	24.04	A	C
ATOM	2123	O	CYS	A	1077	29.738	27.048	0.500	1.00	23.84	A	O
ATOM	2124	N	TRP	A	1078	30.951	25.940	2.042	1.00	24.55	A	N
ATOM	2125	CA	TRP	A	1078	32.224	26.450	1.529	1.00	23.47	A	C
ATOM	2126	CB	TRP	A	1078	33.164	26.849	2.670	1.00	24.02	A	C
ATOM	2127	CG	TRP	A	1078	32.570	27.812	3.646	1.00	23.46	A	C
ATOM	2128	CD2	TRP	A	1078	32.859	27.895	5.042	1.00	23.76	A	C
ATOM	2129	CE2	TRP	A	1078	32.073	28.943	5.571	1.00	23.34	A	C
ATOM	2130	CE3	TRP	A	1078	33.705	27.183	5.901	1.00	21.71	A	C
ATOM	2131	CD1	TRP	A	1078	31.651	28.789	3.386	1.00	24.07	A	C
ATOM	2132	NE1	TRP	A	1078	31.344	29.472	4.537	1.00	24.54	A	N
ATOM	2133	CZ2	TRP	A	1078	32.107	29.300	6.916	1.00	21.87	A	C
ATOM	2134	CZ3	TRP	A	1078	33.737	27.538	7.235	1.00	22.31	A	C
ATOM	2135	CH2	TRP	A	1078	32.942	28.587	7.730	1.00	22.33	A	C
ATOM	2136	C	TRP	A	1078	32.962	25.514	0.594	1.00	23.07	A	C
ATOM	2137	O	TRP	A	1078	34.191	25.455	0.609	1.00	21.26	A	O
ATOM	2138	N	ALA	A	1079	32.216	24.790	−0.229	1.00	24.72	A	N
ATOM	2139	CA	ALA	A	1079	32.837	23.889	−1.190	1.00	26.31	A	C
ATOM	2140	CB	ALA	A	1079	31.791	22.931	−1.788	1.00	25.35	A	C
ATOM	2141	C	ALA	A	1079	33.421	24.768	−2.281	1.00	26.85	A	C
ATOM	2142	O	ALA	A	1079	32.825	25.766	−2.669	1.00	25.36	A	O
ATOM	2143	N	PRO	A	1080	34.602	24.410	−2.791	1.00	28.40	A	N
ATOM	2144	CD	PRO	A	1080	35.464	23.286	−2.388	1.00	27.17	A	C
ATOM	2145	CA	PRO	A	1080	35.228	25.207	−3.848	1.00	29.11	A	C
ATOM	2146	CB	PRO	A	1080	36.371	24.318	−4.318	1.00	27.39	A	C
ATOM	2147	CG	PRO	A	1080	36.780	23.622	−3.072	1.00	27.10	A	C
ATOM	2148	C	PRO	A	1080	34.263	25.547	−4.979	1.00	30.79	A	C
ATOM	2149	O	PRO	A	1080	33.973	26.716	−5.219	1.00	32.38	A	O
ATOM	2150	N	SER	A	1081	33.767	24.521	−5.667	1.00	31.66	A	N
ATOM	2151	CA	SER	A	1081	32.851	24.716	−6.791	1.00	31.24	A	C
ATOM	2152	CB	SER	A	1081	32.873	23.504	−7.724	1.00	35.04	A	C
ATOM	2153	OG	SER	A	1081	32.003	23.698	−8.829	1.00	39.04	A	O
ATOM	2154	C	SER	A	1081	31.427	24.958	−6.345	1.00	28.44	A	C
ATOM	2155	O	SER	A	1081	30.903	24.244	−5.494	1.00	28.65	A	O
ATOM	2156	N	PRO	A	1082	30.775	25.968	−6.939	1.00	26.44	A	N
ATOM	2157	CD	PRO	A	1082	31.403	26.880	−7.908	1.00	25.21	A	C
ATOM	2158	CA	PRO	A	1082	29.397	26.383	−6.667	1.00	26.31	A	C
ATOM	2159	CB	PRO	A	1082	29.188	27.519	−7.655	1.00	23.89	A	C
ATOM	2160	CG	PRO	A	1082	30.552	28.100	−7.783	1.00	24.30	A	C
ATOM	2161	C	PRO	A	1082	28.376	25.264	−6.852	1.00	28.12	A	C
ATOM	2162	O	PRO	A	1082	27.398	25.178	−6.113	1.00	28.72	A	O
ATOM	2163	N	GLN	A	1083	28.604	24.409	−7.839	1.00	28.62	A	N
ATOM	2164	CA	GLN	A	1083	27.691	23.315	−8.095	1.00	31.77	A	C
ATOM	2165	CB	GLN	A	1083	27.953	22.722	−9.477	1.00	36.51	A	C
ATOM	2166	CG	GLN	A	1083	29.425	22.603	−9.827	1.00	43.60	A	C
ATOM	2167	CD	GLN	A	1083	29.670	21.625	−10.960	1.00	48.06	A	C
ATOM	2168	OE1	GLN	A	1083	29.004	21.683	−11.997	1.00	50.45	A	O
ATOM	2169	NE2	GLN	A	1083	30.633	20.721	−10.771	1.00	50.35	A	N
ATOM	2170	C	GLN	A	1083	27.805	22.227	−7.040	1.00	31.92	A	C
ATOM	2171	O	GLN	A	1083	27.016	21.289	−7.031	1.00	30.95	A	O
ATOM	2172	N	ASP	A	1084	28.775	22.350	−6.141	1.00	33.65	A	N
ATOM	2173	CA	ASP	A	1084	28.944	21.336	−5.101	1.00	35.56	A	C
ATOM	2174	CB	ASP	A	1084	30.420	20.927	−4.989	1.00	37.26	A	C
ATOM	2175	CG	ASP	A	1084	30.863	19.995	−6.113	1.00	37.96	A	C
ATOM	2176	OD1	ASP	A	1084	32.049	20.052	−6.502	1.00	39.77	A	O
ATOM	2177	OD2	ASP	A	1084	30.037	19.196	−6.598	1.00	38.93	A	O
ATOM	2178	C	ASP	A	1084	28.406	21.769	−3.733	1.00	34.87	A	C
ATOM	2179	O	ASP	A	1084	28.311	20.954	−2.813	1.00	33.98	A	O
ATOM	2180	N	ARG	A	1085	28.057	23.049	−3.600	1.00	32.96	A	N
ATOM	2181	CA	ARG	A	1085	27.509	23.557	−2.343	1.00	29.33	A	C
ATOM	2182	CB	ARG	A	1085	27.624	25.072	−2.275	1.00	25.99	A	C
ATOM	2183	CG	ARG	A	1085	29.028	25.556	−2.474	1.00	25.88	A	C
ATOM	2184	CD	ARG	A	1085	29.052	27.026	−2.784	1.00	25.19	A	C
ATOM	2185	NE	ARG	A	1085	30.372	27.424	−3.241	1.00	22.90	A	N

TABLE 2-continued

ATOM	2186	CZ	ARG	A	1085	30.617	28.516	−3.949	1.00	23.32	A	C
ATOM	2187	NH1	ARG	A	1085	29.616	29.330	−4.282	1.00	20.28	A	N
ATOM	2188	NH2	ARG	A	1085	31.862	28.770	−4.341	1.00	22.67	A	N
ATOM	2189	C	ARG	A	1085	26.051	23.183	−2.325	1.00	29.39	A	C
ATOM	2190	O	ARG	A	1085	25.404	23.136	−3.369	1.00	30.36	A	O
ATOM	2191	N	PRO	A	1086	25.508	22.908	−1.139	1.00	29.52	A	N
ATOM	2192	CD	PRO	A	1086	26.123	22.945	0.198	1.00	27.74	A	C
ATOM	2193	CA	PRO	A	1086	24.097	22.541	−1.064	1.00	29.00	A	C
ATOM	2194	CB	PRO	A	1086	23.946	22.070	0.375	1.00	29.16	A	C
ATOM	2195	CG	PRO	A	1086	24.918	22.947	1.101	1.00	29.76	A	C
ATOM	2196	C	PRO	A	1086	23.218	23.742	−1.373	1.00	29.28	A	C
ATOM	2197	O	PRO	A	1086	23.659	24.884	−1.287	1.00	30.82	A	O
ATOM	2198	N	SER	A	1087	21.976	23.475	−1.744	1.00	28.64	A	N
ATOM	2199	CA	SER	A	1087	21.040	24.538	−2.048	1.00	29.08	A	C
ATOM	2200	CB	SER	A	1087	19.990	24.048	−3.055	1.00	26.07	A	C
ATOM	2201	OG	SER	A	1087	18.954	23.323	−2.414	1.00	28.14	A	O
ATOM	2202	C	SER	A	1087	20.371	24.936	−0.723	1.00	29.13	A	C
ATOM	2203	O	SER	A	1087	20.535	24.255	0.292	1.00	30.28	A	O
ATOM	2204	N	PHE	A	1088	19.631	26.039	−0.727	1.00	27.78	A	N
ATOM	2205	CA	PHE	A	1088	18.958	26.480	0.476	1.00	27.90	A	C
ATOM	2206	CB	PHE	A	1088	18.426	27.906	0.289	1.00	27.36	A	C
ATOM	2207	CG	PHE	A	1088	19.481	28.974	0.431	1.00	28.07	A	C
ATOM	2208	CD1	PHE	A	1088	19.957	29.337	1.690	1.00	25.93	A	C
ATOM	2209	CD2	PHE	A	1088	20.032	29.586	−0.696	1.00	25.71	A	C
ATOM	2210	CE1	PHE	A	1088	20.960	30.285	1.816	1.00	25.98	A	C
ATOM	2211	CE2	PHE	A	1088	21.035	30.532	−0.580	1.00	24.01	A	C
ATOM	2212	CZ	PHE	A	1088	21.504	30.884	0.675	1.00	24.15	A	C
ATOM	2213	C	PHE	A	1088	17.813	25.527	0.809	1.00	29.45	A	C
ATOM	2214	O	PHE	A	1088	17.482	25.321	1.976	1.00	30.46	A	O
ATOM	2215	N	SER	A	1089	17.217	24.930	−0.216	1.00	29.59	A	N
ATOM	2216	CA	SER	A	1089	16.099	24.025	0.007	1.00	30.75	A	C
ATOM	2217	CB	SER	A	1089	15.436	23.665	−1.315	1.00	30.39	A	C
ATOM	2218	OG	SER	A	1089	16.272	22.786	−2.037	1.00	34.77	A	O
ATOM	2219	C	SER	A	1089	16.581	22.758	0.698	1.00	31.30	A	C
ATOM	2220	O	SER	A	1089	15.834	22.117	1.439	1.00	30.83	A	O
ATOM	2221	N	ALA	A	1090	17.837	22.405	0.445	1.00	31.74	A	N
ATOM	2222	CA	ALA	A	1090	18.444	21.227	1.056	1.00	33.23	A	C
ATOM	2223	CB	ALA	A	1090	19.648	20.771	0.228	1.00	32.69	A	C
ATOM	2224	C	ALA	A	1090	18.874	21.507	2.505	1.00	33.07	A	C
ATOM	2225	O	ALA	A	1090	18.610	20.710	3.399	1.00	33.17	A	O
ATOM	2226	N	LEU	A	1091	19.524	22.644	2.740	1.00	33.22	A	N
ATOM	2227	CA	LEU	A	1091	19.979	22.993	4.089	1.00	33.26	A	C
ATOM	2228	CB	LEU	A	1091	20.848	24.252	4.044	1.00	31.95	A	C
ATOM	2229	CG	LEU	A	1091	22.176	24.091	3.305	1.00	31.49	A	C
ATOM	2230	CD1	LEU	A	1091	22.732	25.436	2.893	1.00	29.88	A	C
ATOM	2231	CD2	LEU	A	1091	23.146	23.352	4.208	1.00	32.95	A	C
ATOM	2232	C	LEU	A	1091	18.819	23.219	5.047	1.00	33.65	A	C
ATOM	2233	O	LEU	A	1091	18.876	22.810	6.210	1.00	33.75	A	O
ATOM	2234	N	GLY	A	1092	17.771	23.869	4.545	1.00	33.60	A	N
ATOM	2235	CA	GLY	A	1092	16.597	24.172	5.350	1.00	33.92	A	C
ATOM	2236	C	GLY	A	1092	16.140	23.084	6.307	1.00	35.32	A	C
ATOM	2237	O	GLY	A	1092	16.383	23.174	7.514	1.00	33.70	A	O
ATOM	2238	N	PRO	A	1093	15.463	22.042	5.798	1.00	35.60	A	N
ATOM	2239	CD	PRO	A	1093	15.256	21.731	4.376	1.00	36.28	A	C
ATOM	2240	CA	PRO	A	1093	14.985	20.949	6.646	1.00	37.04	A	C
ATOM	2241	CB	PRO	A	1093	14.523	19.899	5.633	1.00	37.68	A	C
ATOM	2242	CG	PRO	A	1093	15.311	20.234	4.383	1.00	37.09	A	C
ATOM	2243	C	PRO	A	1093	16.056	20.441	7.610	1.00	38.12	A	C
ATOM	2244	O	PRO	A	1093	15.751	20.082	8.750	1.00	38.30	A	O
ATOM	2245	N	GLN	A	1094	17.309	20.417	7.155	1.00	38.45	A	N
ATOM	2246	CA	GLN	A	1094	18.422	19.992	8.004	1.00	38.71	A	C
ATOM	2247	CB	GLN	A	1094	19.751	20.139	7.264	1.00	39.86	A	C
ATOM	2248	CG	GLN	A	1094	20.135	18.928	6.425	1.00	43.63	A	C
ATOM	2249	CD	GLN	A	1094	20.575	17.740	7.275	1.00	46.77	A	C
ATOM	2250	OE1	GLN	A	1094	19.800	17.213	8.083	1.00	45.34	A	O
ATOM	2251	NE2	GLN	A	1094	21.831	17.317	7.100	1.00	46.94	A	N
ATOM	2252	C	GLN	A	1094	18.442	20.850	9.268	1.00	39.49	A	C
ATOM	2253	O	GLN	A	1094	18.443	20.331	10.385	1.00	39.14	A	O
ATOM	2254	N	LEU	A	1095	18.446	22.168	9.087	1.00	40.38	A	N
ATOM	2255	CA	LEU	A	1095	18.448	23.089	10.220	1.00	40.12	A	C
ATOM	2256	CB	LEU	A	1095	18.596	24.533	9.727	1.00	37.84	A	C
ATOM	2257	CG	LEU	A	1095	19.983	24.906	9.179	1.00	38.91	A	C
ATOM	2258	CD1	LEU	A	1095	19.930	26.219	8.418	1.00	37.27	A	C
ATOM	2259	CD2	LEU	A	1095	20.973	24.992	10.324	1.00	37.75	A	C
ATOM	2260	C	LEU	A	1095	17.180	22.946	11.066	1.00	40.39	A	C
ATOM	2261	O	LEU	A	1095	17.237	22.991	12.296	1.00	38.60	A	O
ATOM	2262	N	ASP	A	1096	16.036	22.773	10.414	1.00	41.84	A	N
ATOM	2263	CA	ASP	A	1096	14.789	22.622	11.153	1.00	44.60	A	C
ATOM	2264	CB	ASP	A	1096	13.633	22.347	10.200	1.00	46.86	A	C
ATOM	2265	CG	ASP	A	1096	12.893	23.603	9.813	1.00	49.73	A	C

TABLE 2-continued

ATOM	2266	OD1	ASP	A	1096	12.144	23.554	8.812	1.00	51.70	A	O
ATOM	2267	OD2	ASP	A	1096	13.058	24.635	10.507	1.00	50.84	A	O
ATOM	2268	C	ASP	A	1096	14.883	21.496	12.172	1.00	44.97	A	C
ATOM	2269	O	ASP	A	1096	14.418	21.637	13.302	1.00	43.90	A	O
ATOM	2270	N	MET	A	1097	15.484	20.381	11.761	1.00	46.10	A	N
ATOM	2271	CA	MET	A	1097	15.649	19.227	12.636	1.00	46.72	A	C
ATOM	2272	CB	MET	A	1097	16.219	18.041	11.863	1.00	49.78	A	C
ATOM	2273	CG	MET	A	1097	15.238	17.360	10.932	1.00	51.99	A	C
ATOM	2274	SD	MET	A	1097	16.001	15.928	10.169	1.00	55.68	A	S
ATOM	2275	CE	MET	A	1097	16.746	16.676	8.742	1.00	54.91	A	C
ATOM	2276	C	MET	A	1097	16.580	19.548	13.788	1.00	46.48	A	C
ATOM	2277	O	MET	A	1097	16.275	19.246	14.938	1.00	47.57	A	O
ATOM	2278	N	LEU	A	1098	17.722	20.149	13.478	1.00	45.27	A	N
ATOM	2279	CA	LEU	A	1098	18.686	20.504	14.508	1.00	45.26	A	C
ATOM	2280	CB	LEU	A	1098	19.872	21.240	13.890	1.00	44.97	A	C
ATOM	2281	CG	LEU	A	1098	20.593	20.490	12.767	1.00	44.21	A	C
ATOM	2282	CD1	LEU	A	1098	21.756	21.322	12.245	1.00	45.02	A	C
ATOM	2283	CD2	LEU	A	1098	21.084	19.150	13.294	1.00	44.66	A	C
ATOM	2284	C	LEU	A	1098	18.031	21.383	15.566	1.00	46.70	A	C
ATOM	2285	O	LEU	A	1098	18.218	21.170	16.768	1.00	46.72	A	O
ATOM	2286	N	TRP	A	1099	17.261	22.367	15.108	1.00	47.34	A	N
ATOM	2287	CA	TRP	A	1099	16.568	23.288	16.003	1.00	47.89	A	C
ATOM	2288	CB	TRP	A	1099	15.587	24.157	15.210	1.00	46.51	A	C
ATOM	2289	CG	TRP	A	1099	14.761	25.053	16.073	1.00	46.41	A	C
ATOM	2290	CD2	TRP	A	1099	13.347	24.974	16.274	1.00	46.89	A	C
ATOM	2291	CE2	TRP	A	1099	12.999	25.985	17.190	1.00	46.27	A	C
ATOM	2292	CE3	TRP	A	1099	12.341	24.144	15.770	1.00	46.19	A	C
ATOM	2293	CD1	TRP	A	1099	15.202	26.085	16.852	1.00	46.39	A	C
ATOM	2294	NE1	TRP	A	1099	14.148	26.649	17.528	1.00	44.71	A	N
ATOM	2295	CZ2	TRP	A	1099	11.691	26.189	17.610	1.00	46.50	A	C
ATOM	2296	CZ3	TRP	A	1099	11.043	24.347	16.189	1.00	45.66	A	C
ATOM	2297	CH2	TRP	A	1099	10.729	25.359	17.100	1.00	46.54	A	C
ATOM	2298	C	TRP	A	1099	15.824	22.527	17.098	1.00	48.58	A	C
ATOM	2299	O	TRP	A	1099	15.812	22.943	18.258	1.00	48.53	A	O
ATOM	2300	N	SER	A	1100	15.210	21.408	16.723	1.00	49.93	A	N
ATOM	2301	CA	SER	A	1100	14.475	20.578	17.673	1.00	51.25	A	C
ATOM	2302	CB	SER	A	1100	13.238	19.965	16.997	1.00	51.15	A	C
ATOM	2303	OG	SER	A	1100	13.586	19.037	15.982	1.00	49.25	A	O
ATOM	2304	C	SER	A	1100	15.375	19.471	18.240	1.00	52.03	A	C
ATOM	2305	O	SER	A	1100	15.541	19.416	19.478	1.00	53.12	A	O
ATOM	2306	OXT	SER	A	1100	15.915	18.674	17.445	1.00	51.89	A	O
TER	1		SER	A	1100						A	
ATOM	2307	CB	ASP	B	813	2.825	23.672	6.637	1.00	41.77	B	C
ATOM	2308	CG	ASP	B	813	1.930	24.126	7.778	1.00	43.25	B	C
ATOM	2309	OD1	ASP	B	813	1.989	23.509	8.863	1.00	45.61	B	O
ATOM	2310	OD2	ASP	B	813	1.169	25.103	7.587	1.00	43.25	B	O
ATOM	2311	C	ASP	B	813	1.324	21.690	6.566	1.00	39.86	B	C
ATOM	2312	O	ASP	B	813	0.396	22.265	5.997	1.00	40.64	B	O
ATOM	2313	N	ASP	B	813	3.241	21.818	5.032	1.00	40.52	B	N
ATOM	2314	CA	ASP	B	813	2.754	22.160	6.398	1.00	40.76	B	C
ATOM	2315	N	PRO	B	814	1.133	20.629	7.357	1.00	38.57	B	N
ATOM	2316	CD	PRO	B	814	2.240	19.827	7.910	1.00	37.96	B	C
ATOM	2317	CA	PRO	B	814	−0.157	20.006	7.657	1.00	36.41	B	C
ATOM	2318	CB	PRO	B	814	0.233	18.772	8.474	1.00	37.07	B	C
ATOM	2319	CG	PRO	B	814	1.617	18.459	8.004	1.00	36.97	B	C
ATOM	2320	C	PRO	B	814	−1.126	20.888	8.433	1.00	35.03	B	C
ATOM	2321	O	PRO	B	814	−0.726	21.746	9.224	1.00	34.82	B	O
ATOM	2322	N	THR	B	815	−2.408	20.645	8.194	1.00	33.52	B	N
ATOM	2323	CA	THR	B	815	−3.495	21.344	8.859	1.00	32.14	B	C
ATOM	2324	CB	THR	B	815	−4.327	22.158	7.862	1.00	31.18	B	C
ATOM	2325	OG1	THR	B	815	−3.534	23.238	7.352	1.00	30.84	B	O
ATOM	2326	CG2	THR	B	815	−5.563	22.711	8.533	1.00	28.45	B	C
ATOM	2327	C	THR	B	815	−4.364	20.247	9.461	1.00	32.63	B	C
ATOM	2328	O	THR	B	815	−5.159	20.484	10.372	1.00	31.96	B	O
ATOM	2329	N	ILE	B	816	−4.178	19.040	8.932	1.00	33.41	B	N
ATOM	2330	CA	ILE	B	816	−4.896	17.842	9.352	1.00	33.58	B	C
ATOM	2331	CB	ILE	B	816	−5.660	17.235	8.164	1.00	35.25	B	C
ATOM	2332	CG2	ILE	B	816	−6.418	15.992	8.595	1.00	37.17	B	C
ATOM	2333	CG1	ILE	B	816	−6.647	18.268	7.622	1.00	37.48	B	C
ATOM	2334	CD1	ILE	B	816	−7.728	18.638	8.595	1.00	34.45	B	C
ATOM	2335	C	ILE	B	816	−3.858	16.846	9.850	1.00	32.05	B	C
ATOM	2336	O	ILE	B	816	−3.011	16.390	9.087	1.00	34.53	B	O
ATOM	2337	N	PHE	B	817	−3.933	16.505	11.128	1.00	29.25	B	N
ATOM	2338	CA	PHE	B	817	−2.967	15.600	11.729	1.00	28.03	B	C
ATOM	2339	CB	PHE	B	817	−2.381	16.230	13.002	1.00	26.53	B	C
ATOM	2340	CG	PHE	B	817	−1.354	17.315	12.743	1.00	22.84	B	C
ATOM	2341	CD1	PHE	B	817	0.001	17.017	12.719	1.00	22.76	B	C
ATOM	2342	CD2	PHE	B	817	−1.744	18.627	12.537	1.00	20.42	B	C
ATOM	2343	CE1	PHE	B	817	0.949	18.013	12.496	1.00	21.47	B	C
ATOM	2344	CE2	PHE	B	817	−0.801	19.628	12.311	1.00	21.52	B	C

TABLE 2-continued

ATOM	2345	CZ	PHE	B	817	0.546	19.319	12.292	1.00	19.38	B	C
ATOM	2346	C	PHE	B	817	−3.543	14.243	12.069	1.00	28.62	B	C
ATOM	2347	O	PHE	B	817	−4.620	14.125	12.661	1.00	28.42	B	O
ATOM	2348	N	GLU	B	818	−2.801	13.212	11.706	1.00	28.25	B	N
ATOM	2349	CA	GLU	B	818	−3.231	11.859	11.976	1.00	30.35	B	C
ATOM	2350	CB	GLU	B	818	−2.673	10.932	10.901	1.00	31.20	B	C
ATOM	2351	CG	GLU	B	818	−3.408	9.624	10.807	1.00	33.27	B	C
ATOM	2352	CD	GLU	B	818	−2.963	8.817	9.632	1.00	34.34	B	C
ATOM	2353	OE1	GLU	B	818	−3.443	7.671	9.498	1.00	35.01	B	O
ATOM	2354	OE2	GLU	B	818	−2.136	9.334	8.849	1.00	33.80	B	O
ATOM	2355	C	GLU	B	818	−2.740	11.430	13.358	1.00	30.11	B	C
ATOM	2356	O	GLU	B	818	−1.557	11.591	13.670	1.00	29.23	B	O
ATOM	2357	N	GLU	B	819	−3.651	10.898	14.178	1.00	28.41	B	N
ATOM	2358	CA	GLU	B	819	−3.326	10.444	15.536	1.00	29.21	B	C
ATOM	2359	CB	GLU	B	819	−4.560	9.853	16.228	1.00	27.11	B	C
ATOM	2360	CG	GLU	B	819	−5.454	10.856	16.963	1.00	26.82	B	C
ATOM	2361	CD	GLU	B	819	−4.707	11.618	18.056	1.00	26.05	B	C
ATOM	2362	OE1	GLU	B	819	−3.821	11.016	18.694	1.00	25.30	B	O
ATOM	2363	OE2	GLU	B	819	−5.010	12.809	18.282	1.00	22.67	B	O
ATOM	2364	C	GLU	B	819	−2.186	9.428	15.630	1.00	31.75	B	C
ATOM	2365	O	GLU	B	819	−1.368	9.499	16.551	1.00	33.63	B	O
ATOM	2366	N	ARG	B	820	−2.120	8.485	14.694	1.00	32.89	B	N
ATOM	2367	CA	ARG	B	820	−1.057	7.488	14.741	1.00	34.85	B	C
ATOM	2368	CB	ARG	B	820	−1.301	6.394	13.685	1.00	37.02	B	C
ATOM	2369	CG	ARG	B	820	−0.780	6.690	12.289	1.00	41.86	B	C
ATOM	2370	CD	ARG	B	820	0.333	5.717	11.892	1.00	46.24	B	C
ATOM	2371	NE	ARG	B	820	1.482	5.810	12.795	1.00	50.85	B	N
ATOM	2372	CZ	ARG	B	820	2.666	5.237	12.587	1.00	51.37	B	C
ATOM	2373	NH1	ARG	B	820	2.884	4.516	11.494	1.00	53.33	B	N
ATOM	2374	NH2	ARG	B	820	3.637	5.387	13.478	1.00	51.30	B	N
ATOM	2375	C	ARG	B	820	0.349	8.107	14.571	1.00	35.30	B	C
ATOM	2376	O	ARG	B	820	1.371	7.455	14.819	1.00	35.40	B	O
ATOM	2377	N	HIS	B	821	0.411	9.368	14.165	1.00	32.42	B	N
ATOM	2378	CA	HIS	B	821	1.706	9.996	13.997	1.00	31.18	B	C
ATOM	2379	CB	HIS	B	821	1.756	10.803	12.695	1.00	32.60	B	C
ATOM	2380	CG	HIS	B	821	1.583	9.969	11.460	1.00	35.70	B	C
ATOM	2381	CD2	HIS	B	821	1.094	10.282	10.235	1.00	35.90	B	C
ATOM	2382	ND1	HIS	B	821	1.964	8.645	11.391	1.00	37.49	B	N
ATOM	2383	CE1	HIS	B	821	1.715	8.177	10.180	1.00	36.47	B	C
ATOM	2384	NE2	HIS	B	821	1.187	9.150	9.461	1.00	37.66	B	N
ATOM	2385	C	HIS	B	821	2.050	10.887	15.184	1.00	30.63	B	C
ATOM	2386	O	HIS	B	821	3.115	11.508	15.215	1.00	30.21	B	O
ATOM	2387	N	LEU	B	822	1.157	10.955	16.166	1.00	28.80	B	N
ATOM	2388	CA	LEU	B	822	1.428	11.776	17.339	1.00	29.94	B	C
ATOM	2389	CB	LEU	B	822	0.172	12.579	17.739	1.00	28.15	B	C
ATOM	2390	CG	LEU	B	822	−0.372	13.555	16.676	1.00	28.24	B	C
ATOM	2391	CD1	LEU	B	822	−1.490	14.423	17.249	1.00	27.85	B	C
ATOM	2392	CD2	LEU	B	822	0.753	14.449	16.184	1.00	27.24	B	C
ATOM	2393	C	LEU	B	822	1.935	10.911	18.508	1.00	30.54	B	C
ATOM	2394	O	LEU	B	822	1.157	10.351	19.269	1.00	29.84	B	O
ATOM	2395	N	LYS	B	823	3.252	10.794	18.638	1.00	31.98	B	N
ATOM	2396	CA	LYS	B	823	3.811	9.987	19.715	1.00	32.61	B	C
ATOM	2397	CB	LYS	B	823	5.234	9.546	19.368	1.00	33.58	B	C
ATOM	2398	CG	LYS	B	823	5.295	8.359	18.418	1.00	36.00	B	C
ATOM	2399	CD	LYS	B	823	4.736	8.690	17.048	1.00	37.37	B	C
ATOM	2400	CE	LYS	B	823	4.240	7.436	16.336	1.00	37.83	B	C
ATOM	2401	NZ	LYS	B	823	5.262	6.364	16.216	1.00	40.50	B	N
ATOM	2402	C	LYS	B	823	3.809	10.698	21.065	1.00	31.17	B	C
ATOM	2403	O	LYS	B	823	4.499	11.696	21.255	1.00	31.27	B	O
ATOM	2404	N	TYR	B	824	3.014	10.178	21.992	1.00	30.97	B	N
ATOM	2405	CA	TYR	B	824	2.922	10.726	23.335	1.00	33.67	B	C
ATOM	2406	CB	TYR	B	824	1.984	9.868	24.184	1.00	34.02	B	C
ATOM	2407	CG	TYR	B	824	2.066	10.155	25.670	1.00	34.31	B	C
ATOM	2408	CD1	TYR	B	824	1.183	11.035	26.276	1.00	34.19	B	C
ATOM	2409	CE1	TYR	B	824	1.253	11.302	27.626	1.00	34.94	B	C
ATOM	2410	CD2	TYR	B	824	3.030	9.549	26.463	1.00	36.32	B	C
ATOM	2411	CE2	TYR	B	824	3.110	9.814	27.821	1.00	37.02	B	C
ATOM	2412	CZ	TYR	B	824	2.216	10.692	28.394	1.00	37.15	B	C
ATOM	2413	OH	TYR	B	824	2.275	10.962	29.746	1.00	39.76	B	O
ATOM	2414	C	TYR	B	824	4.299	10.757	24.010	1.00	34.77	B	C
ATOM	2415	O	TYR	B	824	5.037	9.769	23.988	1.00	31.82	B	O
ATOM	2416	N	ILE	B	825	4.632	11.885	24.626	1.00	35.64	B	N
ATOM	2417	CA	ILE	B	825	5.910	12.004	25.305	1.00	36.01	B	C
ATOM	2418	CB	ILE	B	825	6.751	13.173	24.749	1.00	34.52	B	C
ATOM	2419	CG2	ILE	B	825	8.031	13.325	25.571	1.00	34.43	B	C
ATOM	2420	CG1	ILE	B	825	7.083	12.926	23.275	1.00	33.06	B	C
ATOM	2421	CD1	ILE	B	825	8.072	13.922	22.688	1.00	31.39	B	C
ATOM	2422	C	ILE	B	825	5.711	12.208	26.799	1.00	35.95	B	C
ATOM	2423	O	ILE	B	825	6.537	11.783	27.605	1.00	35.84	B	O
ATOM	2424	N	SER	B	826	4.610	12.853	27.165	1.00	36.03	B	N

TABLE 2-continued

ATOM	2425	CA	SER	B	826	4.303	13.115	28.573	1.00	36.98	B	C
ATOM	2426	CB	SER	B	826	5.507	13.725	29.300	1.00	36.75	B	C
ATOM	2427	OG	SER	B	826	5.831	15.003	28.779	1.00	37.67	B	O
ATOM	2428	C	SER	B	826	3.144	14.082	28.668	1.00	35.86	B	C
ATOM	2429	O	SER	B	826	2.789	14.734	27.688	1.00	37.04	B	O
ATOM	2430	N	GLN	B	827	2.565	14.179	29.857	1.00	36.30	B	N
ATOM	2431	CA	GLN	B	827	1.439	15.073	30.087	1.00	36.00	B	C
ATOM	2432	CB	GLN	B	827	0.463	14.425	31.073	1.00	37.07	B	C
ATOM	2433	CG	GLN	B	827	−0.743	13.784	30.402	1.00	42.24	B	C
ATOM	2434	CD	GLN	B	827	−1.219	12.532	31.120	1.00	46.18	B	C
ATOM	2435	OE1	GLN	B	827	−0.546	11.491	31.104	1.00	47.45	B	O
ATOM	2436	NE2	GLN	B	827	−2.382	12.625	31.759	1.00	47.48	B	N
ATOM	2437	C	GLN	B	827	1.893	16.433	30.609	1.00	34.37	B	C
ATOM	2438	O	GLN	B	827	2.720	16.510	31.521	1.00	33.94	B	O
ATOM	2439	N	LEU	B	828	1.350	17.501	30.023	1.00	32.18	B	N
ATOM	2440	CA	LEU	B	828	1.694	18.862	30.435	1.00	30.39	B	C
ATOM	2441	CB	LEU	B	828	1.616	19.814	29.239	1.00	29.07	B	C
ATOM	2442	CG	LEU	B	828	2.633	19.544	28.133	1.00	27.77	B	C
ATOM	2443	CD1	LEU	B	828	2.337	20.429	26.957	1.00	25.72	B	C
ATOM	2444	CD2	LEU	B	828	4.051	19.780	28.654	1.00	25.98	B	C
ATOM	2445	C	LEU	B	828	0.829	19.401	31.574	1.00	29.13	B	C
ATOM	2446	O	LEU	B	828	1.286	20.229	32.356	1.00	30.42	B	O
ATOM	2447	N	GLY	B	829	−0.412	18.930	31.675	1.00	29.64	B	N
ATOM	2448	CA	GLY	B	829	−1.303	19.384	32.733	1.00	27.62	B	C
ATOM	2449	C	GLY	B	829	−2.758	19.513	32.304	1.00	29.05	B	C
ATOM	2450	O	GLY	B	829	−3.083	19.433	31.115	1.00	29.17	B	O
ATOM	2451	N	LYS	B	830	−3.642	19.706	33.277	1.00	29.83	B	N
ATOM	2452	CA	LYS	B	830	−5.072	19.859	33.018	1.00	29.11	B	C
ATOM	2453	CB	LYS	B	830	−5.867	18.796	33.775	1.00	31.52	B	C
ATOM	2454	CG	LYS	B	830	−7.294	19.234	34.070	1.00	38.23	B	C
ATOM	2455	CD	LYS	B	830	−8.018	18.309	35.034	1.00	41.99	B	C
ATOM	2456	CE	LYS	B	830	−9.305	18.962	35.542	1.00	43.97	B	C
ATOM	2457	NZ	LYS	B	830	−10.060	18.082	36.480	1.00	45.94	B	N
ATOM	2458	C	LYS	B	830	−5.516	21.246	33.489	1.00	27.73	B	C
ATOM	2459	O	LYS	B	830	−5.007	21.744	34.487	1.00	26.97	B	O
ATOM	2460	N	GLY	B	831	−6.457	21.865	32.774	1.00	25.89	B	N
ATOM	2461	CA	GLY	B	831	−6.937	23.182	33.153	1.00	23.83	B	C
ATOM	2462	C	GLY	B	831	−8.447	23.217	33.310	1.00	24.22	B	C
ATOM	2463	O	GLY	B	831	−9.044	22.225	33.717	1.00	24.73	B	O
ATOM	2464	N	ASN	B	832	−9.055	24.353	32.961	1.00	23.96	B	N
ATOM	2465	CA	ASN	B	832	−10.502	24.580	33.046	1.00	21.93	B	C
ATOM	2466	CB	ASN	B	832	−10.804	26.075	33.033	1.00	21.24	B	C
ATOM	2467	CG	ASN	B	832	−10.376	26.770	34.290	1.00	19.88	B	C
ATOM	2468	OD1	ASN	B	832	−10.895	26.475	35.363	1.00	18.71	B	O
ATOM	2469	ND2	ASN	B	832	−9.429	27.710	34.171	1.00	15.25	B	N
ATOM	2470	C	ASN	B	832	−11.351	23.970	31.940	1.00	23.37	B	C
ATOM	2471	O	ASN	B	832	−12.535	23.717	32.151	1.00	22.56	B	O
ATOM	2472	N	PHE	B	833	−10.779	23.772	30.753	1.00	23.17	B	N
ATOM	2473	CA	PHE	B	833	−11.567	23.228	29.647	1.00	24.16	B	C
ATOM	2474	CB	PHE	B	833	−11.790	24.303	28.573	1.00	23.51	B	C
ATOM	2475	CG	PHE	B	833	−12.414	25.567	29.094	1.00	23.24	B	C
ATOM	2476	CD1	PHE	B	833	−11.627	26.641	29.455	1.00	23.38	B	C
ATOM	2477	CD2	PHE	B	833	−13.791	25.675	29.242	1.00	22.46	B	C
ATOM	2478	CE1	PHE	B	833	−12.198	27.808	29.958	1.00	23.81	B	C
ATOM	2479	CE2	PHE	B	833	−14.369	26.842	29.747	1.00	23.47	B	C
ATOM	2480	CZ	PHE	B	833	−13.572	27.905	30.104	1.00	23.00	B	C
ATOM	2481	C	PHE	B	833	−11.005	21.973	28.974	1.00	25.60	B	C
ATOM	2482	O	PHE	B	833	−11.657	21.397	28.106	1.00	25.79	B	O
ATOM	2483	N	GLY	B	834	−9.805	21.548	29.360	1.00	24.96	B	N
ATOM	2484	CA	GLY	B	834	−9.242	20.369	28.746	1.00	24.52	B	C
ATOM	2485	C	GLY	B	834	−7.951	19.924	29.390	1.00	27.71	B	C
ATOM	2486	O	GLY	B	834	−7.689	20.223	30.557	1.00	29.31	B	O
ATOM	2487	N	SER	B	835	−7.149	19.189	28.626	1.00	27.33	B	N
ATOM	2488	CA	SER	B	835	−5.872	18.688	29.096	1.00	28.87	B	C
ATOM	2489	CB	SER	B	835	−6.027	17.258	29.604	1.00	28.44	B	C
ATOM	2490	OG	SER	B	835	−6.763	16.488	28.673	1.00	32.42	B	O
ATOM	2491	C	SER	B	835	−4.888	18.746	27.939	1.00	29.32	B	C
ATOM	2492	O	SER	B	835	−5.280	18.656	26.775	1.00	30.81	B	O
ATOM	2493	N	VAL	B	836	−3.610	18.892	28.263	1.00	28.87	B	N
ATOM	2494	CA	VAL	B	836	−2.573	19.005	27.250	1.00	27.94	B	C
ATOM	2495	CB	VAL	B	836	−1.864	20.358	27.379	1.00	27.26	B	C
ATOM	2496	CG1	VAL	B	836	−0.904	20.560	26.221	1.00	27.80	B	C
ATOM	2497	CG2	VAL	B	836	−2.902	21.478	27.442	1.00	28.52	B	C
ATOM	2498	C	VAL	B	836	−1.525	17.915	27.352	1.00	29.07	B	C
ATOM	2499	O	VAL	B	836	−1.244	17.412	28.437	1.00	30.56	B	O
ATOM	2500	N	GLU	B	837	−0.941	17.556	26.213	1.00	30.14	B	N
ATOM	2501	CA	GLU	B	837	0.101	16.540	26.172	1.00	29.01	B	C
ATOM	2502	CB	GLU	B	837	−0.432	15.215	25.635	1.00	29.10	B	C
ATOM	2503	CG	GLU	B	837	−1.601	14.646	26.378	1.00	28.69	B	C
ATOM	2504	CD	GLU	B	837	−1.757	13.170	26.110	1.00	26.28	B	C

TABLE 2-continued

ATOM	2505	OE1	GLU	B	837	−1.559	12.759	24.949	1.00	26.70	B	O
ATOM	2506	OE2	GLU	B	837	−2.081	12.427	27.054	1.00	25.64	B	O
ATOM	2507	C	GLU	B	837	1.213	16.997	25.252	1.00	29.17	B	C
ATOM	2508	O	GLU	B	837	0.973	17.733	24.293	1.00	27.85	B	O
ATOM	2509	N	LEU	B	838	2.430	16.552	25.564	1.00	30.14	B	N
ATOM	2510	CA	LEU	B	838	3.620	16.858	24.769	1.00	30.84	B	C
ATOM	2511	CB	LEU	B	838	4.837	17.118	25.671	1.00	30.33	B	C
ATOM	2512	CG	LEU	B	838	6.222	17.126	24.999	1.00	31.49	B	C
ATOM	2513	CD1	LEU	B	838	6.315	18.235	23.951	1.00	31.48	B	C
ATOM	2514	CD2	LEU	B	838	7.303	17.315	26.059	1.00	30.64	B	C
ATOM	2515	C	LEU	B	838	3.876	15.628	23.917	1.00	30.49	B	C
ATOM	2516	O	LEU	B	838	4.277	14.587	24.433	1.00	32.32	B	O
ATOM	2517	N	CYS	B	839	3.624	15.742	22.619	1.00	29.82	B	N
ATOM	2518	CA	CYS	B	839	3.819	14.627	21.700	1.00	29.62	B	C
ATOM	2519	CB	CYS	B	839	2.521	14.304	20.960	1.00	26.21	B	C
ATOM	2520	SG	CYS	B	839	1.103	14.029	21.990	1.00	25.86	B	S
ATOM	2521	C	CYS	B	839	4.867	14.972	20.655	1.00	30.35	B	C
ATOM	2522	O	CYS	B	839	5.418	16.069	20.646	1.00	29.37	B	O
ATOM	2523	N	ARG	B	840	5.138	14.023	19.769	1.00	32.26	B	N
ATOM	2524	CA	ARG	B	840	6.083	14.272	18.692	1.00	35.32	B	C
ATOM	2525	CB	ARG	B	840	7.361	13.442	18.879	1.00	36.76	B	C
ATOM	2526	CG	ARG	B	840	8.401	13.640	17.780	1.00	39.60	B	C
ATOM	2527	CD	ARG	B	840	9.699	12.899	18.083	1.00	42.80	B	C
ATOM	2528	NE	ARG	B	840	10.542	13.641	19.019	1.00	44.90	B	N
ATOM	2529	CZ	ARG	B	840	11.121	13.129	20.104	1.00	45.26	B	C
ATOM	2530	NH1	ARG	B	840	10.964	11.845	20.421	1.00	44.02	B	N
ATOM	2531	NH2	ARG	B	840	11.847	13.921	20.883	1.00	44.63	B	N
ATOM	2532	C	ARG	B	840	5.393	13.908	17.384	1.00	34.75	B	C
ATOM	2533	O	ARG	B	840	4.787	12.841	17.273	1.00	33.34	B	O
ATOM	2534	N	TYR	B	841	5.446	14.817	16.413	1.00	36.29	B	N
ATOM	2535	CA	TYR	B	841	4.832	14.566	15.116	1.00	39.08	B	C
ATOM	2536	CB	TYR	B	841	4.463	15.877	14.407	1.00	38.47	B	C
ATOM	2537	CG	TYR	B	841	3.756	15.674	13.079	1.00	39.29	B	C
ATOM	2538	CD1	TYR	B	841	2.737	14.736	12.950	1.00	38.25	B	C
ATOM	2539	CE1	TYR	B	841	2.092	14.538	11.743	1.00	37.76	B	C
ATOM	2540	CD2	TYR	B	841	4.109	16.416	11.956	1.00	39.45	B	C
ATOM	2541	CE2	TYR	B	841	3.467	16.228	10.741	1.00	38.84	B	C
ATOM	2542	CZ	TYR	B	841	2.458	15.285	10.642	1.00	39.62	B	C
ATOM	2543	OH	TYR	B	841	1.809	15.084	9.441	1.00	40.43	B	O
ATOM	2544	C	TYR	B	841	5.890	13.820	14.345	1.00	41.24	B	C
ATOM	2545	O	TYR	B	841	6.773	14.420	13.753	1.00	42.10	B	O
ATOM	2546	N	ASP	B	842	5.793	12.497	14.362	1.00	44.63	B	N
ATOM	2547	CA	ASP	B	842	6.781	11.662	13.711	1.00	46.51	B	C
ATOM	2548	CB	ASP	B	842	7.449	10.796	14.779	1.00	45.68	B	C
ATOM	2549	CG	ASP	B	842	8.819	10.324	14.369	1.00	45.45	B	C
ATOM	2550	OD1	ASP	B	842	9.593	11.153	13.849	1.00	44.25	B	O
ATOM	2551	OD2	ASP	B	842	9.124	9.130	14.579	1.00	44.55	B	O
ATOM	2552	C	ASP	B	842	6.237	10.787	12.586	1.00	48.84	B	C
ATOM	2553	O	ASP	B	842	6.237	9.558	12.688	1.00	49.65	B	O
ATOM	2554	N	PRO	B	843	5.773	11.412	11.491	1.00	51.03	B	N
ATOM	2555	CD	PRO	B	843	5.703	12.871	11.295	1.00	51.92	B	C
ATOM	2556	CA	PRO	B	843	5.228	10.700	10.330	1.00	52.68	B	C
ATOM	2557	CB	PRO	B	843	5.019	11.814	9.310	1.00	52.46	B	C
ATOM	2558	CG	PRO	B	843	4.709	12.999	10.165	1.00	52.25	B	C
ATOM	2559	C	PRO	B	843	6.197	9.628	9.819	1.00	54.74	B	C
ATOM	2560	O	PRO	B	843	5.793	8.688	9.141	1.00	55.91	B	O
ATOM	2561	N	LEU	B	844	7.478	9.780	10.145	1.00	56.20	B	N
ATOM	2562	CA	LEU	B	844	8.497	8.820	9.730	1.00	58.07	B	C
ATOM	2563	CB	LEU	B	844	9.699	9.555	9.133	1.00	58.51	B	C
ATOM	2564	CG	LEU	B	844	9.416	10.518	7.974	1.00	59.43	B	C
ATOM	2565	CD1	LEU	B	844	8.650	9.777	6.893	1.00	58.93	B	C
ATOM	2566	CD2	LEU	B	844	8.610	11.715	8.455	1.00	59.39	B	C
ATOM	2567	C	LEU	B	844	8.941	8.003	10.945	1.00	59.20	B	C
ATOM	2568	O	LEU	B	844	8.979	8.516	12.060	1.00	60.38	B	O
ATOM	2569	N	GLY	B	845	9.274	6.735	10.728	1.00	60.38	B	N
ATOM	2570	CA	GLY	B	845	9.694	5.882	11.826	1.00	60.46	B	C
ATOM	2571	C	GLY	B	845	10.727	6.510	12.740	1.00	61.81	B	C
ATOM	2572	O	GLY	B	845	10.627	6.417	13.966	1.00	62.35	B	O
ATOM	2573	N	ASP	B	846	11.725	7.149	12.138	1.00	61.41	B	N
ATOM	2574	CA	ASP	B	846	12.796	7.801	12.880	1.00	61.12	B	C
ATOM	2575	CB	ASP	B	846	13.815	8.393	11.902	1.00	63.52	B	C
ATOM	2576	CG	ASP	B	846	13.163	9.224	10.804	1.00	64.79	B	C
ATOM	2577	OD1	ASP	B	846	13.865	9.584	9.833	1.00	65.93	B	O
ATOM	2578	OD2	ASP	B	846	11.953	9.520	10.910	1.00	66.12	B	O
ATOM	2579	C	ASP	B	846	12.252	8.893	13.788	1.00	60.47	B	C
ATOM	2580	O	ASP	B	846	11.215	9.476	13.501	1.00	61.57	B	O
ATOM	2581	N	ASN	B	847	12.958	9.174	14.877	1.00	59.01	B	N
ATOM	2582	CA	ASN	B	847	12.530	10.199	15.827	1.00	56.87	B	C
ATOM	2583	CB	ASN	B	847	13.062	9.863	17.214	1.00	58.01	B	C
ATOM	2584	CG	ASN	B	847	12.536	8.551	17.722	1.00	58.36	B	C

TABLE 2-continued

ATOM	2585	OD1	ASN	B	847	11.474	8.494	18.341	1.00	58.73	B	O
ATOM	2586	ND2	ASN	B	847	13.265	7.475	17.441	1.00	58.76	B	N
ATOM	2587	C	ASN	B	847	13.005	11.588	15.442	1.00	54.91	B	C
ATOM	2588	O	ASN	B	847	13.483	12.343	16.289	1.00	54.35	B	O
ATOM	2589	N	THR	B	848	12.870	11.924	14.167	1.00	52.24	B	N
ATOM	2590	CA	THR	B	848	13.299	13.226	13.684	1.00	51.03	B	C
ATOM	2591	CB	THR	B	848	13.704	13.157	12.214	1.00	50.95	B	C
ATOM	2592	OG1	THR	B	848	12.547	12.871	11.419	1.00	50.21	B	O
ATOM	2593	CG2	THR	B	848	14.738	12.069	12.004	1.00	50.33	B	C
ATOM	2594	C	THR	B	848	12.199	14.272	13.817	1.00	49.92	B	C
ATOM	2595	O	THR	B	848	12.481	15.465	13.911	1.00	49.66	B	O
ATOM	2596	N	GLY	B	849	10.950	13.817	13.820	1.00	47.29	B	N
ATOM	2597	CA	GLY	B	849	9.817	14.722	13.923	1.00	44.59	B	C
ATOM	2598	C	GLY	B	849	9.944	15.813	14.969	1.00	41.66	B	C
ATOM	2599	O	GLY	B	849	10.759	15.708	15.881	1.00	41.89	B	O
ATOM	2600	N	ALA	B	850	9.125	16.855	14.835	1.00	40.04	B	N
ATOM	2601	CA	ALA	B	850	9.124	17.993	15.755	1.00	37.64	B	C
ATOM	2602	CB	ALA	B	850	8.782	19.269	14.993	1.00	37.63	B	C
ATOM	2603	C	ALA	B	850	8.163	17.831	16.931	1.00	36.65	B	C
ATOM	2604	O	ALA	B	850	7.197	17.067	16.869	1.00	35.41	B	O
ATOM	2605	N	LEU	B	851	8.432	18.566	18.005	1.00	35.80	B	N
ATOM	2606	CA	LEU	B	851	7.581	18.515	19.189	1.00	35.03	B	C
ATOM	2607	CB	LEU	B	851	8.384	18.865	20.440	1.00	36.07	B	C
ATOM	2608	CG	LEU	B	851	9.620	18.013	20.740	1.00	38.49	B	C
ATOM	2609	CD1	LEU	B	851	10.456	18.721	21.792	1.00	38.97	B	C
ATOM	2610	CD2	LEU	B	851	9.214	16.630	21.219	1.00	38.23	B	C
ATOM	2611	C	LEU	B	851	6.429	19.501	19.045	1.00	32.82	B	C
ATOM	2612	O	LEU	B	851	6.566	20.529	18.386	1.00	32.71	B	O
ATOM	2613	N	VAL	B	852	5.293	19.179	19.658	1.00	30.52	B	N
ATOM	2614	CA	VAL	B	852	4.124	20.054	19.619	1.00	28.26	B	C
ATOM	2615	CB	VAL	B	852	3.228	19.804	18.360	1.00	28.68	B	C
ATOM	2616	CG1	VAL	B	852	3.906	20.344	17.105	1.00	28.83	B	C
ATOM	2617	CG2	VAL	B	852	2.923	18.315	18.212	1.00	26.07	B	C
ATOM	2618	C	VAL	B	852	3.251	19.850	20.852	1.00	27.93	B	C
ATOM	2619	O	VAL	B	852	3.344	18.832	21.537	1.00	27.53	B	O
ATOM	2620	N	ALA	B	853	2.407	20.826	21.147	1.00	26.02	B	N
ATOM	2621	CA	ALA	B	853	1.504	20.680	22.269	1.00	25.71	B	C
ATOM	2622	CB	ALA	B	853	1.305	21.998	22.946	1.00	25.74	B	C
ATOM	2623	C	ALA	B	853	0.178	20.181	21.694	1.00	27.28	B	C
ATOM	2624	O	ALA	B	853	−0.270	20.650	20.642	1.00	26.81	B	O
ATOM	2625	N	VAL	B	854	−0.446	19.223	22.371	1.00	26.44	B	N
ATOM	2626	CA	VAL	B	854	−1.719	18.704	21.897	1.00	26.10	B	C
ATOM	2627	CB	VAL	B	854	−1.603	17.240	21.464	1.00	24.99	B	C
ATOM	2628	CG1	VAL	B	854	−2.890	16.797	20.801	1.00	26.57	B	C
ATOM	2629	CG2	VAL	B	854	−0.433	17.074	20.509	1.00	25.76	B	C
ATOM	2630	C	VAL	B	854	−2.793	18.817	22.971	1.00	26.92	B	C
ATOM	2631	O	VAL	B	854	−2.791	18.068	23.945	1.00	27.18	B	O
ATOM	2632	N	LYS	B	855	−3.709	19.766	22.798	1.00	26.33	B	N
ATOM	2633	CA	LYS	B	855	−4.775	19.934	23.768	1.00	25.94	B	C
ATOM	2634	CB	LYS	B	855	−5.015	21.409	24.084	1.00	22.34	B	C
ATOM	2635	CG	LYS	B	855	−6.335	21.613	24.811	1.00	23.65	B	C
ATOM	2636	CD	LYS	B	855	−6.706	23.063	25.021	1.00	19.73	B	C
ATOM	2637	CE	LYS	B	855	−5.997	23.682	26.197	1.00	17.77	B	C
ATOM	2638	NZ	LYS	B	855	−6.896	24.693	26.805	1.00	15.49	B	N
ATOM	2639	C	LYS	B	855	−6.089	19.321	23.300	1.00	26.94	B	C
ATOM	2640	O	LYS	B	855	−6.501	19.506	22.159	1.00	26.18	B	O
ATOM	2641	N	GLN	B	856	−6.732	18.577	24.196	1.00	29.24	B	N
ATOM	2642	CA	GLN	B	856	−8.021	17.964	23.919	1.00	29.00	B	C
ATOM	2643	CB	GLN	B	856	−7.965	16.456	24.152	1.00	29.02	B	C
ATOM	2644	CG	GLN	B	856	−9.299	15.739	23.913	1.00	31.97	B	C
ATOM	2645	CD	GLN	B	856	−9.154	14.220	23.867	1.00	33.49	B	C
ATOM	2646	OE1	GLN	B	856	−8.570	13.613	24.764	1.00	37.69	B	O
ATOM	2647	NE2	GLN	B	856	−9.682	13.603	22.818	1.00	31.47	B	N
ATOM	2648	C	GLN	B	856	−9.026	18.598	24.875	1.00	30.25	B	C
ATOM	2649	O	GLN	B	856	−8.826	18.596	26.089	1.00	30.29	B	O
ATOM	2650	N	LEU	B	857	−10.096	19.152	24.320	1.00	32.05	B	N
ATOM	2651	CA	LEU	B	857	−11.135	19.793	25.116	1.00	34.93	B	C
ATOM	2652	CB	LEU	B	857	−11.879	20.828	24.259	1.00	32.54	B	C
ATOM	2653	CG	LEU	B	857	−11.173	22.161	23.971	1.00	32.83	B	C
ATOM	2654	CD1	LEU	B	857	−9.699	21.937	23.781	1.00	34.65	B	C
ATOM	2655	CD2	LEU	B	857	−11.765	22.817	22.733	1.00	32.44	B	C
ATOM	2656	C	LEU	B	857	−12.133	18.779	25.670	1.00	37.68	B	C
ATOM	2657	O	LEU	B	857	−12.298	17.689	25.125	1.00	35.98	B	O
ATOM	2658	N	GLN	B	858	−12.771	19.135	26.778	1.00	41.97	B	N
ATOM	2659	CA	GLN	B	858	−13.785	18.285	27.377	1.00	48.02	B	C
ATOM	2660	CB	GLN	B	858	−14.058	18.705	28.820	1.00	49.27	B	C
ATOM	2661	CG	GLN	B	858	−15.107	17.856	29.506	1.00	53.78	B	C
ATOM	2662	CD	GLN	B	858	−15.374	18.277	30.942	1.00	56.64	B	C
ATOM	2663	OE1	GLN	B	858	−14.453	18.366	31.764	1.00	57.31	B	O
ATOM	2664	NE2	GLN	B	858	−16.643	18.533	31.254	1.00	56.69	B	N

TABLE 2-continued

ATOM	2665	C	GLN	B	858	−15.009	18.565	26.518	1.00	51.34	B	C
ATOM	2666	O	GLN	B	858	−15.540	19.678	26.516	1.00	51.97	B	O
ATOM	2667	N	HIS	B	859	−15.451	17.564	25.774	1.00	55.49	B	N
ATOM	2668	CA	HIS	B	859	−16.585	17.750	24.888	1.00	59.37	B	C
ATOM	2669	CB	HIS	B	859	−16.117	17.622	23.434	1.00	60.01	B	C
ATOM	2670	CG	HIS	B	859	−17.057	18.227	22.438	1.00	61.60	B	C
ATOM	2671	CD2	HIS	B	859	−16.825	19.001	21.352	1.00	61.93	B	C
ATOM	2672	ND1	HIS	B	859	−18.419	18.026	22.482	1.00	62.55	B	N
ATOM	2673	CE1	HIS	B	859	−18.987	18.650	21.465	1.00	62.95	B	C
ATOM	2674	NE2	HIS	B	859	−18.042	19.248	20.764	1.00	63.01	B	N
ATOM	2675	C	HIS	B	859	−17.670	16.728	25.172	1.00	61.41	B	C
ATOM	2676	O	HIS	B	859	−17.551	15.563	24.791	1.00	62.79	B	O
ATOM	2677	N	SER	B	860	−18.725	17.160	25.850	1.00	63.19	B	N
ATOM	2678	CA	SER	B	860	−19.830	16.262	26.158	1.00	64.59	B	C
ATOM	2679	CB	SER	B	860	−20.137	16.266	27.658	1.00	65.49	B	C
ATOM	2680	OG	SER	B	860	−19.100	15.632	28.388	1.00	65.65	B	O
ATOM	2681	C	SER	B	860	−21.061	16.671	25.369	1.00	65.19	B	C
ATOM	2682	O	SER	B	860	−21.907	17.428	25.847	1.00	65.42	B	O
ATOM	2683	N	GLY	B	861	−21.133	16.161	24.145	1.00	65.17	B	N
ATOM	2684	CA	GLY	B	861	−22.241	16.438	23.252	1.00	64.91	B	C
ATOM	2685	C	GLY	B	861	−21.825	15.917	21.892	1.00	64.88	B	C
ATOM	2686	O	GLY	B	861	−20.727	15.374	21.771	1.00	65.32	B	O
ATOM	2687	N	PRO	B	862	−22.664	16.039	20.854	1.00	64.29	B	N
ATOM	2688	CD	PRO	B	862	−23.978	16.696	20.759	1.00	64.63	B	C
ATOM	2689	CA	PRO	B	862	−22.231	15.533	19.547	1.00	63.09	B	C
ATOM	2690	CB	PRO	B	862	−23.435	15.824	18.649	1.00	63.47	B	C
ATOM	2691	CG	PRO	B	862	−24.050	17.029	19.291	1.00	63.98	B	C
ATOM	2692	C	PRO	B	862	−20.954	16.244	19.082	1.00	61.34	B	C
ATOM	2693	O	PRO	B	862	−20.909	17.471	18.994	1.00	60.26	B	O
ATOM	2694	N	ASP	B	863	−19.913	15.464	18.815	1.00	59.65	B	N
ATOM	2695	CA	ASP	B	863	−18.641	16.013	18.361	1.00	57.84	B	C
ATOM	2696	CB	ASP	B	863	−17.621	14.898	18.145	1.00	59.72	B	C
ATOM	2697	CG	ASP	B	863	−17.906	14.092	16.885	1.00	59.59	B	C
ATOM	2698	OD1	ASP	B	863	−19.027	13.543	16.778	1.00	60.44	B	O
ATOM	2699	OD2	ASP	B	863	−17.017	14.015	16.007	1.00	58.51	B	O
ATOM	2700	C	ASP	B	863	−18.911	16.660	17.023	1.00	55.52	B	C
ATOM	2701	O	ASP	B	863	−19.630	16.097	16.202	1.00	56.67	B	O
ATOM	2702	N	GLN	B	864	−18.340	17.833	16.790	1.00	50.93	B	N
ATOM	2703	CA	GLN	B	864	−18.553	18.496	15.518	1.00	45.49	B	C
ATOM	2704	CB	GLN	B	864	−19.307	19.798	15.720	1.00	48.68	B	C
ATOM	2705	CG	GLN	B	864	−20.798	19.572	15.845	1.00	51.79	B	C
ATOM	2706	CD	GLN	B	864	−21.292	18.598	14.792	1.00	53.83	B	C
ATOM	2707	OE1	GLN	B	864	−21.023	18.775	13.597	1.00	55.56	B	O
ATOM	2708	NE2	GLN	B	864	−22.013	17.561	15.224	1.00	52.86	B	N
ATOM	2709	C	GLN	B	864	−17.254	18.738	14.782	1.00	40.84	B	C
ATOM	2710	O	GLN	B	864	−16.640	19.798	14.890	1.00	40.71	B	O
ATOM	2711	N	GLN	B	865	−16.852	17.725	14.029	1.00	34.97	B	N
ATOM	2712	CA	GLN	B	865	−15.629	17.754	13.266	1.00	31.61	B	C
ATOM	2713	CB	GLN	B	865	−15.589	16.516	12.378	1.00	28.65	B	C
ATOM	2714	CG	GLN	B	865	−14.437	16.458	11.410	1.00	27.56	B	C
ATOM	2715	CD	GLN	B	865	−14.698	17.265	10.155	1.00	26.59	B	C
ATOM	2716	OE1	GLN	B	865	−15.741	17.111	9.508	1.00	24.08	B	O
ATOM	2717	NE2	GLN	B	865	−13.747	18.126	9.797	1.00	25.55	B	N
ATOM	2718	C	GLN	B	865	−15.479	19.035	12.445	1.00	30.61	B	C
ATOM	2719	O	GLN	B	865	−14.467	19.735	12.552	1.00	28.62	B	O
ATOM	2720	N	ARG	B	866	−16.490	19.339	11.638	1.00	29.87	B	N
ATOM	2721	CA	ARG	B	866	−16.476	20.532	10.800	1.00	28.92	B	C
ATOM	2722	CB	ARG	B	866	−17.797	20.668	10.040	1.00	29.98	B	C
ATOM	2723	CG	ARG	B	866	−17.936	19.702	8.876	1.00	32.46	B	C
ATOM	2724	CD	ARG	B	866	−19.170	20.020	8.056	1.00	31.87	B	C
ATOM	2725	NE	ARG	B	866	−20.035	18.859	7.879	1.00	34.46	B	N
ATOM	2726	CZ	ARG	B	866	−19.936	17.987	6.881	1.00	33.51	B	C
ATOM	2727	NH1	ARG	B	866	−19.005	18.129	5.948	1.00	33.94	B	N
ATOM	2728	NH2	ARG	B	866	−20.783	16.974	6.806	1.00	30.60	B	N
ATOM	2729	C	ARG	B	866	−16.196	21.805	11.596	1.00	27.94	B	C
ATOM	2730	O	ARG	B	866	−15.380	22.623	11.182	1.00	25.73	B	O
ATOM	2731	N	ASP	B	867	−16.869	21.978	12.730	1.00	29.03	B	N
ATOM	2732	CA	ASP	B	867	−16.635	23.151	13.566	1.00	30.85	B	C
ATOM	2733	CB	ASP	B	867	−17.448	23.070	14.859	1.00	32.87	B	C
ATOM	2734	CG	ASP	B	867	−18.942	23.283	14.630	1.00	36.23	B	C
ATOM	2735	OD1	ASP	B	867	−19.339	24.352	14.103	1.00	36.54	B	O
ATOM	2736	OD2	ASP	B	867	−19.726	22.376	14.985	1.00	38.32	B	O
ATOM	2737	C	ASP	B	867	−15.157	23.296	13.904	1.00	30.96	B	C
ATOM	2738	O	ASP	B	867	−14.558	24.329	13.599	1.00	31.28	B	O
ATOM	2739	N	PHE	B	868	−14.571	22.267	14.526	1.00	32.13	B	N
ATOM	2740	CA	PHE	B	868	−13.148	22.297	14.894	1.00	31.94	B	C
ATOM	2741	CB	PHE	B	868	−12.675	20.940	15.446	1.00	29.88	B	C
ATOM	2742	CG	PHE	B	868	−13.005	20.707	16.896	1.00	27.56	B	C
ATOM	2743	CD1	PHE	B	868	−14.312	20.517	17.306	1.00	26.67	B	C
ATOM	2744	CD2	PHE	B	868	−11.999	20.675	17.852	1.00	28.33	B	C

TABLE 2-continued

ATOM	2745	CE1	PHE	B	868	−14.612	20.301	18.648	1.00	27.39	B	C
ATOM	2746	CE2	PHE	B	868	−12.289	20.461	19.196	1.00	27.40	B	C
ATOM	2747	CZ	PHE	B	868	−13.596	20.275	19.595	1.00	25.66	B	C
ATOM	2748	C	PHE	B	868	−12.312	22.627	13.662	1.00	32.28	B	C
ATOM	2749	O	PHE	B	868	−11.351	23.389	13.722	1.00	33.97	B	O
ATOM	2750	N	GLN	B	869	−12.688	22.038	12.540	1.00	32.23	B	N
ATOM	2751	CA	GLN	B	869	−11.974	22.249	11.291	1.00	32.63	B	C
ATOM	2752	CB	GLN	B	869	−12.571	21.327	10.223	1.00	33.42	B	C
ATOM	2753	CG	GLN	B	869	−11.852	21.318	8.896	1.00	38.59	B	C
ATOM	2754	CD	GLN	B	869	−10.454	20.729	8.970	1.00	42.27	B	C
ATOM	2755	OE1	GLN	B	869	−9.720	20.742	7.982	1.00	45.09	B	O
ATOM	2756	NE2	GLN	B	869	−10.078	20.209	10.135	1.00	42.53	B	N
ATOM	2757	C	GLN	B	869	−12.056	23.713	10.850	1.00	31.04	B	C
ATOM	2758	O	GLN	B	869	−11.073	24.300	10.398	1.00	31.14	B	O
ATOM	2759	N	ARG	B	870	−13.232	24.303	11.002	1.00	29.80	B	N
ATOM	2760	CA	ARG	B	870	−13.453	25.684	10.600	1.00	28.79	B	C
ATOM	2761	CB	ARG	B	870	−14.947	26.016	10.751	1.00	28.73	B	C
ATOM	2762	CG	ARG	B	870	−15.346	27.449	10.417	1.00	29.41	B	C
ATOM	2763	CD	ARG	B	870	−16.761	27.746	10.889	1.00	26.01	B	C
ATOM	2764	NE	ARG	B	870	−16.875	27.628	12.338	1.00	24.89	B	N
ATOM	2765	CZ	ARG	B	870	−17.761	26.859	12.960	1.00	26.54	B	C
ATOM	2766	NH1	ARG	B	870	−18.624	26.129	12.258	1.00	23.91	B	N
ATOM	2767	NH2	ARG	B	870	−17.780	26.815	14.288	1.00	23.42	B	N
ATOM	2768	C	ARG	B	870	−12.602	26.657	11.415	1.00	28.20	B	C
ATOM	2769	O	ARG	B	870	−11.893	27.492	10.857	1.00	27.89	B	O
ATOM	2770	N	GLU	B	871	−12.670	26.535	12.735	1.00	28.44	B	N
ATOM	2771	CA	GLU	B	871	−11.932	27.416	13.629	1.00	29.10	B	C
ATOM	2772	CB	GLU	B	871	−12.327	27.110	15.073	1.00	28.98	B	C
ATOM	2773	CG	GLU	B	871	−13.821	27.293	15.330	1.00	27.67	B	C
ATOM	2774	CD	GLU	B	871	−14.295	28.709	15.029	1.00	30.59	B	C
ATOM	2775	OE1	GLU	B	871	−15.422	28.862	14.501	1.00	28.93	B	O
ATOM	2776	OE2	GLU	B	871	−13.542	29.668	15.326	1.00	29.15	B	O
ATOM	2777	C	GLU	B	871	−10.414	27.353	13.454	1.00	30.42	B	C
ATOM	2778	O	GLU	B	871	−9.746	28.386	13.315	1.00	29.98	B	O
ATOM	2779	N	ILE	B	872	−9.864	26.147	13.448	1.00	30.79	B	N
ATOM	2780	CA	ILE	B	872	−8.426	26.001	13.283	1.00	32.19	B	C
ATOM	2781	CB	ILE	B	872	−8.012	24.524	13.279	1.00	33.29	B	C
ATOM	2782	CG2	ILE	B	872	−6.888	24.301	12.305	1.00	34.00	B	C
ATOM	2783	CG1	ILE	B	872	−7.572	24.114	14.678	1.00	33.72	B	C
ATOM	2784	CD1	ILE	B	872	−6.373	24.849	15.148	1.00	29.33	B	C
ATOM	2785	C	ILE	B	872	−7.916	26.662	12.012	1.00	32.54	B	C
ATOM	2786	O	ILE	B	872	−6.819	27.215	11.997	1.00	34.61	B	O
ATOM	2787	N	GLN	B	873	−8.696	26.609	10.936	1.00	32.00	B	N
ATOM	2788	CA	GLN	B	873	−8.253	27.234	9.697	1.00	29.37	B	C
ATOM	2789	CB	GLN	B	873	−9.112	26.785	8.516	1.00	30.42	B	C
ATOM	2790	CG	GLN	B	873	−9.011	25.305	8.255	1.00	33.60	B	C
ATOM	2791	CD	GLN	B	873	−9.613	24.874	6.935	1.00	36.54	B	C
ATOM	2792	OE1	GLN	B	873	−9.545	23.695	6.584	1.00	40.58	B	O
ATOM	2793	NE2	GLN	B	873	−10.202	25.820	6.193	1.00	36.08	B	N
ATOM	2794	C	GLN	B	873	−8.316	28.741	9.845	1.00	28.83	B	C
ATOM	2795	O	GLN	B	873	−7.571	29.471	9.189	1.00	27.50	B	O
ATOM	2796	N	ILE	B	874	−9.213	29.201	10.714	1.00	26.87	B	N
ATOM	2797	CA	ILE	B	874	−9.365	30.627	10.971	1.00	26.03	B	C
ATOM	2798	CB	ILE	B	874	−10.718	30.939	11.681	1.00	25.77	B	C
ATOM	2799	CG2	ILE	B	874	−10.687	32.326	12.277	1.00	25.42	B	C
ATOM	2800	CG1	ILE	B	874	−11.874	30.854	10.690	1.00	24.44	B	C
ATOM	2801	CD1	ILE	B	874	−13.199	31.183	11.296	1.00	25.79	B	C
ATOM	2802	C	ILE	B	874	−8.216	31.066	11.875	1.00	27.22	B	C
ATOM	2803	O	ILE	B	874	−7.586	32.106	11.648	1.00	26.87	B	O
ATOM	2804	N	LEU	B	875	−7.947	30.251	12.898	1.00	27.62	B	N
ATOM	2805	CA	LEU	B	875	−6.886	30.535	13.859	1.00	25.96	B	C
ATOM	2806	CB	LEU	B	875	−7.024	29.638	15.099	1.00	24.59	B	C
ATOM	2807	CG	LEU	B	875	−8.270	29.838	15.983	1.00	24.64	B	C
ATOM	2808	CD1	LEU	B	875	−8.328	28.786	17.075	1.00	22.44	B	C
ATOM	2809	CD2	LEU	B	875	−8.248	31.208	16.601	1.00	24.13	B	C
ATOM	2810	C	LEU	B	875	−5.510	30.377	13.228	1.00	26.34	B	C
ATOM	2811	O	LEU	B	875	−4.621	31.206	13.439	1.00	27.82	B	O
ATOM	2812	N	LYS	B	876	−5.328	29.335	12.430	1.00	25.15	B	N
ATOM	2813	CA	LYS	B	876	−4.034	29.145	11.796	1.00	25.86	B	C
ATOM	2814	CB	LYS	B	876	−4.012	27.832	11.022	1.00	24.63	B	C
ATOM	2815	CG	LYS	B	876	−2.646	27.477	10.473	1.00	24.05	B	C
ATOM	2816	CD	LYS	B	876	−2.659	26.077	9.898	1.00	23.72	B	C
ATOM	2817	CE	LYS	B	876	−1.280	25.687	9.445	1.00	23.59	B	C
ATOM	2818	NZ	LYS	B	876	−1.240	24.405	8.706	1.00	24.88	B	N
ATOM	2819	C	LYS	B	876	−3.648	30.307	10.866	1.00	26.99	B	C
ATOM	2820	O	LYS	B	876	−2.461	30.594	10.689	1.00	29.84	B	O
ATOM	2821	N	ALA	B	877	−4.634	30.973	10.269	1.00	26.24	B	N
ATOM	2822	CA	ALA	B	877	−4.350	32.100	9.377	1.00	27.52	B	C
ATOM	2823	CB	ALA	B	877	−5.592	32.435	8.548	1.00	26.74	B	C
ATOM	2824	C	ALA	B	877	−3.858	33.352	10.144	1.00	28.24	B	C

TABLE 2-continued

ATOM	2825	O	ALA	B	877	−3.229	34.229	9.569	1.00	27.71	B	O
ATOM	2826	N	LEU	B	878	−4.140	33.428	11.442	1.00	30.40	B	N
ATOM	2827	CA	LEU	B	878	−3.702	34.561	12.266	1.00	29.17	B	C
ATOM	2828	CB	LEU	B	878	−4.304	34.452	13.656	1.00	27.14	B	C
ATOM	2829	CG	LEU	B	878	−5.822	34.321	13.719	1.00	27.92	B	C
ATOM	2830	CD1	LEU	B	878	−6.218	33.768	15.073	1.00	27.76	B	C
ATOM	2831	CD2	LEU	B	878	−6.465	35.663	13.458	1.00	26.98	B	C
ATOM	2832	C	LEU	B	878	−2.186	34.521	12.383	1.00	29.28	B	C
ATOM	2833	O	LEU	B	878	−1.619	33.457	12.610	1.00	28.90	B	O
ATOM	2834	N	HIS	B	879	−1.536	35.672	12.237	1.00	30.42	B	N
ATOM	2835	CA	HIS	B	879	−0.081	35.741	12.321	1.00	31.74	B	C
ATOM	2836	CB	HIS	B	879	0.514	35.780	10.925	1.00	32.65	B	C
ATOM	2837	CG	HIS	B	879	0.386	34.489	10.186	1.00	37.56	B	C
ATOM	2838	CD2	HIS	B	879	0.520	33.208	10.602	1.00	39.16	B	C
ATOM	2839	ND1	HIS	B	879	0.112	34.426	8.837	1.00	39.12	B	N
ATOM	2840	CE1	HIS	B	879	0.083	33.163	8.453	1.00	39.56	B	C
ATOM	2841	NE2	HIS	B	879	0.328	32.405	9.506	1.00	41.59	B	N
ATOM	2842	C	HIS	B	879	0.459	36.918	13.125	1.00	32.27	B	C
ATOM	2843	O	HIS	B	879	0.257	38.076	12.762	1.00	32.06	B	O
ATOM	2844	N	SER	B	880	1.165	36.597	14.207	1.00	30.30	B	N
ATOM	2845	CA	SER	B	880	1.767	37.590	15.091	1.00	30.83	B	C
ATOM	2846	CB	SER	B	880	0.720	38.147	16.062	1.00	29.12	B	C
ATOM	2847	OG	SER	B	880	1.336	38.938	17.063	1.00	25.06	B	O
ATOM	2848	C	SER	B	880	2.923	36.964	15.882	1.00	31.96	B	C
ATOM	2849	O	SER	B	880	2.840	35.818	16.334	1.00	32.79	B	O
ATOM	2850	N	ASP	B	881	4.003	37.711	16.053	1.00	31.67	B	N
ATOM	2851	CA	ASP	B	881	5.131	37.172	16.786	1.00	31.34	B	C
ATOM	2852	CB	ASP	B	881	6.346	38.069	16.642	1.00	34.15	B	C
ATOM	2853	CG	ASP	B	881	6.976	37.961	15.283	1.00	38.28	B	C
ATOM	2854	OD1	ASP	B	881	8.035	38.584	15.081	1.00	41.45	B	O
ATOM	2855	OD2	ASP	B	881	6.414	37.258	14.416	1.00	40.35	B	O
ATOM	2856	C	ASP	B	881	4.806	37.010	18.249	1.00	28.71	B	C
ATOM	2857	O	ASP	B	881	5.532	36.346	18.977	1.00	26.63	B	O
ATOM	2858	N	PHE	B	882	3.709	37.618	18.681	1.00	26.82	B	N
ATOM	2859	CA	PHE	B	882	3.319	37.526	20.081	1.00	25.00	B	C
ATOM	2860	CB	PHE	B	882	3.045	38.923	20.628	1.00	25.06	B	C
ATOM	2861	CG	PHE	B	882	4.170	39.886	20.397	1.00	25.00	B	C
ATOM	2862	CD1	PHE	B	882	5.431	39.631	20.899	1.00	26.44	B	C
ATOM	2863	CD2	PHE	B	882	3.979	41.021	19.631	1.00	27.51	B	C
ATOM	2864	CE1	PHE	B	882	6.491	40.492	20.636	1.00	27.79	B	C
ATOM	2865	CE2	PHE	B	882	5.030	41.884	19.365	1.00	27.41	B	C
ATOM	2866	CZ	PHE	B	882	6.287	41.620	19.866	1.00	25.41	B	C
ATOM	2867	C	PHE	B	882	2.093	36.630	20.254	1.00	23.95	B	C
ATOM	2868	O	PHE	B	882	1.238	36.892	21.092	1.00	24.37	B	O
ATOM	2869	N	ILE	B	883	2.033	35.561	19.463	1.00	23.06	B	N
ATOM	2870	CA	ILE	B	883	0.921	34.616	19.492	1.00	23.35	B	C
ATOM	2871	CB	ILE	B	883	−0.083	34.904	18.339	1.00	25.35	B	C
ATOM	2872	CG2	ILE	B	883	−0.362	33.652	17.546	1.00	25.61	B	C
ATOM	2873	CG1	ILE	B	883	−1.378	35.470	18.907	1.00	24.93	B	C
ATOM	2874	CD1	ILE	B	883	−1.239	36.865	19.365	1.00	23.61	B	C
ATOM	2875	C	ILE	B	883	1.430	33.190	19.351	1.00	22.62	B	C
ATOM	2876	O	ILE	B	883	2.351	32.917	18.587	1.00	19.13	B	O
ATOM	2877	N	VAL	B	884	0.842	32.276	20.105	1.00	24.11	B	N
ATOM	2878	CA	VAL	B	884	1.257	30.881	20.025	1.00	24.99	B	C
ATOM	2879	CB	VAL	B	884	0.836	30.129	21.289	1.00	25.13	B	C
ATOM	2880	CG1	VAL	B	884	1.339	28.699	21.232	1.00	24.82	B	C
ATOM	2881	CG2	VAL	B	884	1.361	30.859	22.520	1.00	27.61	B	C
ATOM	2882	C	VAL	B	884	0.595	30.252	18.792	1.00	24.61	B	C
ATOM	2883	O	VAL	B	884	−0.627	30.199	18.698	1.00	23.23	B	O
ATOM	2884	N	LYS	B	885	1.415	29.783	17.857	1.00	25.26	B	N
ATOM	2885	CA	LYS	B	885	0.929	29.198	16.612	1.00	25.39	B	C
ATOM	2886	CB	LYS	B	885	2.100	28.837	15.702	1.00	25.63	B	C
ATOM	2887	CG	LYS	B	885	3.023	29.989	15.351	1.00	28.38	B	C
ATOM	2888	CD	LYS	B	885	4.276	29.480	14.643	1.00	30.17	B	C
ATOM	2889	CE	LYS	B	885	5.217	30.615	14.293	1.00	32.49	B	C
ATOM	2890	NZ	LYS	B	885	4.547	31.591	13.381	1.00	35.37	B	N
ATOM	2891	C	LYS	B	885	0.058	27.968	16.751	1.00	25.44	B	C
ATOM	2892	O	LYS	B	885	0.393	27.036	17.469	1.00	26.56	B	O
ATOM	2893	N	TYR	B	886	−1.073	27.982	16.063	1.00	25.34	B	N
ATOM	2894	CA	TYR	B	886	−1.954	26.833	16.045	1.00	25.02	B	C
ATOM	2895	CB	TYR	B	886	−3.417	27.277	15.944	1.00	25.04	B	C
ATOM	2896	CG	TYR	B	886	−4.100	27.564	17.274	1.00	21.78	B	C
ATOM	2897	CD1	TYR	B	886	−4.291	26.560	18.220	1.00	20.76	B	C
ATOM	2898	CE1	TYR	B	886	−4.962	26.809	19.403	1.00	18.65	B	C
ATOM	2899	CD2	TYR	B	886	−4.597	28.820	17.556	1.00	20.53	B	C
ATOM	2900	CE2	TYR	B	886	−5.266	29.075	18.728	1.00	20.17	B	C
ATOM	2901	CZ	TYR	B	886	−5.447	28.074	19.648	1.00	19.43	B	C
ATOM	2902	OH	TYR	B	886	−6.118	28.366	20.815	1.00	17.53	B	O
ATOM	2903	C	TYR	B	886	−1.508	26.123	14.768	1.00	24.51	B	C
ATOM	2904	O	TYR	B	886	−1.266	26.772	13.743	1.00	22.88	B	O

TABLE 2-continued

ATOM	2905	N	ARG	B	887	−1.378	24.803	14.818	1.00	24.90	B	N
ATOM	2906	CA	ARG	B	887	−0.916	24.070	13.645	1.00	24.72	B	C
ATOM	2907	CB	ARG	B	887	0.283	23.199	14.016	1.00	25.16	B	C
ATOM	2908	CG	ARG	B	887	1.551	23.983	14.248	1.00	27.60	B	C
ATOM	2909	CD	ARG	B	887	2.733	23.042	14.379	1.00	30.25	B	C
ATOM	2910	NE	ARG	B	887	2.962	22.287	13.154	1.00	31.62	B	N
ATOM	2911	CZ	ARG	B	887	3.892	21.349	13.023	1.00	32.40	B	C
ATOM	2912	NH1	ARG	B	887	4.674	21.054	14.046	1.00	34.33	B	N
ATOM	2913	NH2	ARG	B	887	4.049	20.710	11.869	1.00	33.94	B	N
ATOM	2914	C	ARG	B	887	−1.946	23.220	12.919	1.00	23.82	B	C
ATOM	2915	O	ARG	B	887	−1.855	23.047	11.706	1.00	24.22	B	O
ATOM	2916	N	GLY	B	888	−2.916	22.681	13.649	1.00	23.86	B	N
ATOM	2917	CA	GLY	B	888	−3.923	21.852	13.011	1.00	22.84	B	C
ATOM	2918	C	GLY	B	888	−4.841	21.140	13.984	1.00	23.38	B	C
ATOM	2919	O	GLY	B	888	−4.868	21.450	15.182	1.00	23.89	B	O
ATOM	2920	N	VAL	B	889	−5.594	20.181	13.448	1.00	21.47	B	N
ATOM	2921	CA	VAL	B	889	−6.543	19.373	14.210	1.00	21.70	B	C
ATOM	2922	CB	VAL	B	889	−7.998	19.607	13.725	1.00	20.93	B	C
ATOM	2923	CG1	VAL	B	889	−8.921	18.534	14.281	1.00	19.14	B	C
ATOM	2924	CG2	VAL	B	889	−8.471	20.966	14.169	1.00	23.06	B	C
ATOM	2925	C	VAL	B	889	−6.221	17.898	14.012	1.00	21.52	B	C
ATOM	2926	O	VAL	B	889	−5.950	17.462	12.900	1.00	22.29	B	O
ATOM	2927	N	SER	B	890	−6.276	17.117	15.080	1.00	22.47	B	N
ATOM	2928	CA	SER	B	890	−5.966	15.705	14.945	1.00	24.44	B	C
ATOM	2929	CB	SER	B	890	−5.233	15.195	16.183	1.00	21.47	B	C
ATOM	2930	OG	SER	B	890	−6.168	14.893	17.203	1.00	23.05	B	O
ATOM	2931	C	SER	B	890	−7.228	14.875	14.745	1.00	26.17	B	C
ATOM	2932	O	SER	B	890	−8.289	15.185	15.291	1.00	27.00	B	O
ATOM	2933	N	TYR	B	891	−7.105	13.820	13.948	1.00	27.10	B	N
ATOM	2934	CA	TYR	B	891	−8.223	12.926	13.708	1.00	27.93	B	C
ATOM	2935	CB	TYR	B	891	−8.644	12.987	12.243	1.00	27.86	B	C
ATOM	2936	CG	TYR	B	891	−9.260	14.312	11.916	1.00	30.15	B	C
ATOM	2937	CD1	TYR	B	891	−10.480	14.672	12.447	1.00	31.47	B	C
ATOM	2938	CE1	TYR	B	891	−11.015	15.912	12.216	1.00	30.53	B	C
ATOM	2939	CD2	TYR	B	891	−8.594	15.231	11.140	1.00	27.69	B	C
ATOM	2940	CE2	TYR	B	891	−9.118	16.468	10.905	1.00	28.64	B	C
ATOM	2941	CZ	TYR	B	891	−10.329	16.809	11.447	1.00	29.64	B	C
ATOM	2942	OH	TYR	B	891	−10.851	18.069	11.246	1.00	30.89	B	O
ATOM	2943	C	TYR	B	891	−7.863	11.506	14.116	1.00	28.23	B	C
ATOM	2944	O	TYR	B	891	−6.875	10.943	13.648	1.00	25.30	B	O
ATOM	2945	N	GLY	B	892	−8.698	10.956	14.992	1.00	30.66	B	N
ATOM	2946	CA	GLY	B	892	−8.548	9.619	15.539	1.00	35.15	B	C
ATOM	2947	C	GLY	B	892	−8.159	8.464	14.652	1.00	36.94	B	C
ATOM	2948	O	GLY	B	892	−7.194	8.567	13.900	1.00	40.72	B	O
ATOM	2949	N	PRO	B	893	−8.865	7.326	14.752	1.00	37.28	B	N
ATOM	2950	CD	PRO	B	893	−8.482	6.075	14.068	1.00	37.20	B	C
ATOM	2951	CA	PRO	B	893	−9.997	7.096	15.655	1.00	37.62	B	C
ATOM	2952	CB	PRO	B	893	−10.583	5.791	15.135	1.00	37.35	B	C
ATOM	2953	CG	PRO	B	893	−9.338	5.035	14.768	1.00	38.08	B	C
ATOM	2954	C	PRO	B	893	−9.597	6.973	17.124	1.00	37.60	B	C
ATOM	2955	O	PRO	B	893	−8.594	7.546	17.585	1.00	37.03	B	O
ATOM	2956	N	GLY	B	894	−10.392	6.201	17.851	1.00	35.38	B	N
ATOM	2957	CA	GLY	B	894	−10.121	6.004	19.262	1.00	33.52	B	C
ATOM	2958	C	GLY	B	894	−10.552	7.189	20.100	1.00	31.99	B	C
ATOM	2959	O	GLY	B	894	−11.030	8.188	19.565	1.00	29.77	B	O
ATOM	2960	N	ARG	B	895	−10.383	7.070	21.417	1.00	32.32	B	N
ATOM	2961	CA	ARG	B	895	−10.753	8.122	22.365	1.00	30.91	B	C
ATOM	2962	CB	ARG	B	895	−10.360	7.722	23.797	1.00	32.42	B	C
ATOM	2963	CG	ARG	B	895	−11.237	6.645	24.398	1.00	35.42	B	C
ATOM	2964	CD	ARG	B	895	−10.720	6.093	25.744	1.00	37.59	B	C
ATOM	2965	NE	ARG	B	895	−10.850	7.020	26.866	1.00	38.06	B	N
ATOM	2966	CZ	ARG	B	895	−9.883	7.830	27.285	1.00	41.12	B	C
ATOM	2967	NH1	ARG	B	895	−8.699	7.829	26.676	1.00	40.31	B	N
ATOM	2968	NH2	ARG	B	895	−10.105	8.641	28.313	1.00	40.07	B	N
ATOM	2969	C	ARG	B	895	−10.109	9.460	22.032	1.00	28.48	B	C
ATOM	2970	O	ARG	B	895	−10.770	10.496	22.077	1.00	27.31	B	O
ATOM	2971	N	GLN	B	896	−8.826	9.452	21.695	1.00	26.23	B	N
ATOM	2972	CA	GLN	B	896	−8.167	10.711	21.397	1.00	27.50	B	C
ATOM	2973	CB	GLN	B	896	−6.704	10.671	21.852	1.00	26.61	B	C
ATOM	2974	CG	GLN	B	896	−6.539	10.509	23.361	1.00	21.98	B	C
ATOM	2975	CD	GLN	B	896	−5.128	10.816	23.834	1.00	23.58	B	C
ATOM	2976	OE1	GLN	B	896	−4.150	10.290	23.298	1.00	26.22	B	O
ATOM	2977	NE2	GLN	B	896	−5.015	11.667	24.845	1.00	21.74	B	N
ATOM	2978	C	GLN	B	896	−8.248	11.133	19.941	1.00	28.56	B	C
ATOM	2979	O	GLN	B	896	−7.594	10.558	19.074	1.00	31.99	B	O
ATOM	2980	N	SER	B	897	−9.051	12.158	19.679	1.00	28.29	B	N
ATOM	2981	CA	SER	B	897	−9.218	12.678	18.327	1.00	26.97	B	C
ATOM	2982	CB	SER	B	897	−10.161	11.770	17.532	1.00	26.11	B	C
ATOM	2983	OG	SER	B	897	−10.161	12.129	16.162	1.00	24.03	B	O
ATOM	2984	C	SER	B	897	−9.767	14.113	18.357	1.00	26.27	B	C

TABLE 2-continued

ATOM	2985	O	SER	B	897	−10.235	14.587	19.392	1.00	24.86	B	O
ATOM	2986	N	LEU	B	898	−9.722	14.798	17.219	1.00	25.36	B	N
ATOM	2987	CA	LEU	B	898	−10.204	16.170	17.160	1.00	26.00	B	C
ATOM	2988	CB	LEU	B	898	−11.723	16.216	17.341	1.00	26.02	B	C
ATOM	2989	CG	LEU	B	898	−12.565	15.882	16.108	1.00	24.07	B	C
ATOM	2990	CD1	LEU	B	898	−14.011	15.662	16.510	1.00	23.90	B	C
ATOM	2991	CD2	LEU	B	898	−12.459	17.016	15.113	1.00	24.33	B	C
ATOM	2992	C	LEU	B	898	−9.530	17.007	18.242	1.00	26.30	B	C
ATOM	2993	O	LEU	B	898	−10.170	17.830	18.888	1.00	28.60	B	O
ATOM	2994	N	ARG	B	899	−8.234	16.779	18.437	1.00	25.95	B	N
ATOM	2995	CA	ARG	B	899	−7.457	17.516	19.425	1.00	24.40	B	C
ATOM	2996	CB	ARG	B	899	−6.443	16.595	20.114	1.00	22.59	B	C
ATOM	2997	CG	ARG	B	899	−7.058	15.350	20.727	1.00	22.64	B	C
ATOM	2998	CD	ARG	B	899	−6.076	14.637	21.641	1.00	23.58	B	C
ATOM	2999	NE	ARG	B	899	−4.855	14.240	20.951	1.00	23.78	B	N
ATOM	3000	CZ	ARG	B	899	−3.763	13.805	21.570	1.00	24.40	B	C
ATOM	3001	NH1	ARG	B	899	−2.696	13.461	20.868	1.00	26.08	B	N
ATOM	3002	NH2	ARG	B	899	−3.727	13.730	22.890	1.00	23.65	B	N
ATOM	3003	C	ARG	B	899	−6.731	18.659	18.711	1.00	24.37	B	C
ATOM	3004	O	ARG	B	899	−6.476	18.601	17.509	1.00	25.32	B	O
ATOM	3005	N	LEU	B	900	−6.394	19.693	19.461	1.00	22.83	B	N
ATOM	3006	CA	LEU	B	900	−5.736	20.848	18.901	1.00	22.29	B	C
ATOM	3007	CB	LEU	B	900	−6.203	22.095	19.673	1.00	23.06	B	C
ATOM	3008	CG	LEU	B	900	−7.727	22.284	19.877	1.00	18.99	B	C
ATOM	3009	CD1	LEU	B	900	−8.021	23.367	20.901	1.00	20.49	B	C
ATOM	3010	CD2	LEU	B	900	−8.369	22.632	18.564	1.00	20.01	B	C
ATOM	3011	C	LEU	B	900	−4.218	20.681	18.980	1.00	23.70	B	C
ATOM	3012	O	LEU	B	900	−3.663	20.403	20.047	1.00	24.33	B	O
ATOM	3013	N	VAL	B	901	−3.552	20.839	17.841	1.00	24.29	B	N
ATOM	3014	CA	VAL	B	901	−2.102	20.713	17.765	1.00	23.11	B	C
ATOM	3015	CB	VAL	B	901	−1.679	19.896	16.508	1.00	23.04	B	C
ATOM	3016	CG1	VAL	B	901	−0.170	19.702	16.485	1.00	16.20	B	C
ATOM	3017	CG2	VAL	B	901	−2.396	18.538	16.500	1.00	21.11	B	C
ATOM	3018	C	VAL	B	901	−1.499	22.113	17.677	1.00	24.80	B	C
ATOM	3019	O	VAL	B	901	−1.844	22.890	16.790	1.00	25.60	B	O
ATOM	3020	N	MET	B	902	−0.587	22.433	18.587	1.00	26.09	B	N
ATOM	3021	CA	MET	B	902	0.026	23.752	18.591	1.00	25.58	B	C
ATOM	3022	CB	MET	B	902	−0.412	24.530	19.822	1.00	26.88	B	C
ATOM	3023	CG	MET	B	902	−1.878	24.456	20.127	1.00	27.85	B	C
ATOM	3024	SD	MET	B	902	−2.092	24.944	21.814	1.00	28.15	B	S
ATOM	3025	CE	MET	B	902	−2.056	23.354	22.644	1.00	23.45	B	C
ATOM	3026	C	MET	B	902	1.533	23.636	18.650	1.00	25.59	B	C
ATOM	3027	O	MET	B	902	2.072	22.556	18.912	1.00	24.38	B	O
ATOM	3028	N	GLU	B	903	2.205	24.762	18.420	1.00	24.65	B	N
ATOM	3029	CA	GLU	B	903	3.650	24.798	18.509	1.00	26.30	B	C
ATOM	3030	CB	GLU	B	903	4.199	26.136	17.987	1.00	25.66	B	C
ATOM	3031	CG	GLU	B	903	3.970	27.328	18.910	1.00	27.57	B	C
ATOM	3032	CD	GLU	B	903	4.572	28.629	18.381	1.00	26.55	B	C
ATOM	3033	OE1	GLU	B	903	5.638	28.581	17.728	1.00	25.12	B	O
ATOM	3034	OE2	GLU	B	903	3.980	29.699	18.638	1.00	25.41	B	O
ATOM	3035	C	GLU	B	903	3.910	24.651	20.010	1.00	26.13	B	C
ATOM	3036	O	GLU	B	903	3.087	25.068	20.830	1.00	28.56	B	O
ATOM	3037	N	TYR	B	904	5.039	24.058	20.369	1.00	24.40	B	N
ATOM	3038	CA	TYR	B	904	5.384	23.840	21.769	1.00	24.74	B	C
ATOM	3039	CB	TYR	B	904	5.891	22.409	21.921	1.00	23.92	B	C
ATOM	3040	CG	TYR	B	904	6.433	22.085	23.289	1.00	24.77	B	C
ATOM	3041	CD1	TYR	B	904	5.590	21.959	24.379	1.00	24.64	B	C
ATOM	3042	CE1	TYR	B	904	6.084	21.600	25.613	1.00	24.42	B	C
ATOM	3043	CD2	TYR	B	904	7.791	21.852	23.480	1.00	24.71	B	C
ATOM	3044	CE2	TYR	B	904	8.291	21.492	24.706	1.00	22.58	B	C
ATOM	3045	CZ	TYR	B	904	7.435	21.363	25.766	1.00	23.33	B	C
ATOM	3046	OH	TYR	B	904	7.932	20.953	26.978	1.00	25.34	B	O
ATOM	3047	C	TYR	B	904	6.433	24.809	22.340	1.00	24.37	B	C
ATOM	3048	O	TYR	B	904	7.525	24.950	21.780	1.00	23.11	B	O
ATOM	3049	N	LEU	B	905	6.097	25.470	23.448	1.00	23.71	B	N
ATOM	3050	CA	LEU	B	905	7.025	26.394	24.113	1.00	23.78	B	C
ATOM	3051	CB	LEU	B	905	6.398	27.770	24.306	1.00	23.71	B	C
ATOM	3052	CG	LEU	B	905	6.535	28.734	23.124	1.00	24.68	B	C
ATOM	3053	CD1	LEU	B	905	5.750	28.211	21.936	1.00	22.49	B	C
ATOM	3054	CD2	LEU	B	905	6.026	30.119	23.541	1.00	23.69	B	C
ATOM	3055	C	LEU	B	905	7.372	25.823	25.470	1.00	23.58	B	C
ATOM	3056	O	LEU	B	905	6.633	26.026	26.429	1.00	24.54	B	O
ATOM	3057	N	PRO	B	906	8.513	25.114	25.568	1.00	24.82	B	N
ATOM	3058	CD	PRO	B	906	9.481	25.084	24.457	1.00	26.24	B	C
ATOM	3059	CA	PRO	B	906	9.080	24.443	26.743	1.00	26.73	B	C
ATOM	3060	CB	PRO	B	906	10.366	23.822	26.191	1.00	26.64	B	C
ATOM	3061	CG	PRO	B	906	10.787	24.789	25.168	1.00	25.89	B	C
ATOM	3062	C	PRO	B	906	9.316	25.248	28.024	1.00	28.44	B	C
ATOM	3063	O	PRO	B	906	9.476	24.663	29.098	1.00	31.05	B	O
ATOM	3064	N	SER	B	907	9.338	26.571	27.938	1.00	27.81	B	N

TABLE 2-continued

ATOM	3065	CA	SER	B	907	9.552	27.360	29.143	1.00	25.91	B	C
ATOM	3066	CB	SER	B	907	10.091	28.739	28.793	1.00	25.32	B	C
ATOM	3067	OG	SER	B	907	11.451	28.635	28.422	1.00	25.14	B	O
ATOM	3068	C	SER	B	907	8.319	27.486	30.024	1.00	24.89	B	C
ATOM	3069	O	SER	B	907	8.420	27.921	31.164	1.00	25.08	B	O
ATOM	3070	N	GLY	B	908	7.153	27.115	29.504	1.00	24.02	B	N
ATOM	3071	CA	GLY	B	908	5.949	27.173	30.318	1.00	23.21	B	C
ATOM	3072	C	GLY	B	908	5.254	28.513	30.404	1.00	23.91	B	C
ATOM	3073	O	GLY	B	908	5.668	29.485	29.762	1.00	23.15	B	O
ATOM	3074	N	CYS	B	909	4.199	28.565	31.220	1.00	23.69	B	N
ATOM	3075	CA	CYS	B	909	3.405	29.783	31.391	1.00	24.23	B	C
ATOM	3076	CB	CYS	B	909	2.080	29.468	32.097	1.00	23.91	B	C
ATOM	3077	SG	CYS	B	909	2.192	28.992	33.844	1.00	26.62	B	S
ATOM	3078	C	CYS	B	909	4.116	30.922	32.116	1.00	25.56	B	C
ATOM	3079	O	CYS	B	909	5.124	30.722	32.781	1.00	28.14	B	O
ATOM	3080	N	LEU	B	910	3.575	32.126	31.994	1.00	25.80	B	N
ATOM	3081	CA	LEU	B	910	4.187	33.280	32.612	1.00	25.97	B	C
ATOM	3082	CB	LEU	B	910	3.703	34.555	31.928	1.00	25.51	B	C
ATOM	3083	CG	LEU	B	910	4.255	35.889	32.424	1.00	21.94	B	C
ATOM	3084	CD1	LEU	B	910	5.764	35.900	32.325	1.00	19.02	B	C
ATOM	3085	CD2	LEU	B	910	3.651	37.004	31.588	1.00	21.42	B	C
ATOM	3086	C	LEU	B	910	3.841	33.319	34.075	1.00	27.73	B	C
ATOM	3087	O	LEU	B	910	4.581	33.882	34.872	1.00	29.03	B	O
ATOM	3088	N	ARG	B	911	2.710	32.718	34.423	1.00	29.17	B	N
ATOM	3089	CA	ARG	B	911	2.261	32.677	35.804	1.00	30.07	B	C
ATOM	3090	CB	ARG	B	911	0.955	31.886	35.907	1.00	30.79	B	C
ATOM	3091	CG	ARG	B	911	0.360	31.832	37.299	1.00	31.95	B	C
ATOM	3092	CD	ARG	B	911	0.525	30.472	37.965	1.00	35.46	B	C
ATOM	3093	NE	ARG	B	911	−0.638	29.607	37.749	1.00	37.85	B	N
ATOM	3094	CZ	ARG	B	911	−0.706	28.645	36.831	1.00	37.82	B	C
ATOM	3095	NH1	ARG	B	911	0.336	28.414	36.039	1.00	37.46	B	N
ATOM	3096	NH2	ARG	B	911	−1.819	27.924	36.696	1.00	34.64	B	N
ATOM	3097	C	ARG	B	911	3.329	32.051	36.692	1.00	31.19	B	C
ATOM	3098	O	ARG	B	911	3.693	32.627	37.711	1.00	31.62	B	O
ATOM	3099	N	ASP	B	912	3.842	30.886	36.298	1.00	31.73	B	N
ATOM	3100	CA	ASP	B	912	4.870	30.195	37.081	1.00	32.01	B	C
ATOM	3101	CB	ASP	B	912	4.969	28.732	36.654	1.00	31.15	B	C
ATOM	3102	CG	ASP	B	912	3.686	27.962	36.903	1.00	33.95	B	C
ATOM	3103	OD1	ASP	B	912	3.597	26.796	36.461	1.00	37.34	B	O
ATOM	3104	OD2	ASP	B	912	2.768	28.515	37.542	1.00	35.80	B	O
ATOM	3105	C	ASP	B	912	6.244	30.846	36.946	1.00	32.72	B	C
ATOM	3106	O	ASP	B	912	7.044	30.842	37.886	1.00	35.14	B	O
ATOM	3107	N	PHE	B	913	6.512	31.396	35.768	1.00	30.42	B	N
ATOM	3108	CA	PHE	B	913	7.781	32.047	35.493	1.00	27.92	B	C
ATOM	3109	CB	PHE	B	913	7.789	32.552	34.057	1.00	27.63	B	C
ATOM	3110	CG	PHE	B	913	9.131	32.976	33.575	1.00	24.31	B	C
ATOM	3111	CD1	PHE	B	913	10.023	32.041	33.077	1.00	25.48	B	C
ATOM	3112	CD2	PHE	B	913	9.498	34.313	33.601	1.00	25.91	B	C
ATOM	3113	CE1	PHE	B	913	11.270	32.427	32.604	1.00	25.71	B	C
ATOM	3114	CE2	PHE	B	913	10.741	34.717	33.133	1.00	26.67	B	C
ATOM	3115	CZ	PHE	B	913	11.632	33.769	32.630	1.00	26.64	B	C
ATOM	3116	C	PHE	B	913	7.969	33.228	36.439	1.00	28.84	B	C
ATOM	3117	O	PHE	B	913	9.021	33.396	37.061	1.00	28.01	B	O
ATOM	3118	N	LEU	B	914	6.941	34.059	36.525	1.00	28.32	B	N
ATOM	3119	CA	LEU	B	914	6.989	35.217	37.389	1.00	28.91	B	C
ATOM	3120	CB	LEU	B	914	5.641	35.944	37.369	1.00	26.17	B	C
ATOM	3121	CG	LEU	B	914	5.350	36.893	36.203	1.00	25.31	B	C
ATOM	3122	CD1	LEU	B	914	3.852	37.120	36.120	1.00	23.40	B	C
ATOM	3123	CD2	LEU	B	914	6.086	38.217	36.391	1.00	21.60	B	C
ATOM	3124	C	LEU	B	914	7.351	34.839	38.823	1.00	30.29	B	C
ATOM	3125	O	LEU	B	914	8.151	35.518	39.461	1.00	31.24	B	O
ATOM	3126	N	GLN	B	915	6.778	33.750	39.322	1.00	30.78	B	N
ATOM	3127	CA	GLN	B	915	7.036	33.326	40.695	1.00	31.85	B	C
ATOM	3128	CB	GLN	B	915	6.017	32.263	41.107	1.00	28.47	B	C
ATOM	3129	CG	GLN	B	915	4.599	32.792	41.121	1.00	26.27	B	C
ATOM	3130	CD	GLN	B	915	3.551	31.705	41.216	1.00	27.48	B	C
ATOM	3131	OE1	GLN	B	915	2.756	31.690	42.143	1.00	28.95	B	O
ATOM	3132	NE2	GLN	B	915	3.545	30.791	40.253	1.00	29.42	B	N
ATOM	3133	C	GLN	B	915	8.453	32.817	40.943	1.00	32.63	B	C
ATOM	3134	O	GLN	B	915	9.059	33.123	41.962	1.00	31.97	B	O
ATOM	3135	N	ARG	B	916	8.980	32.049	40.008	1.00	35.56	B	N
ATOM	3136	CA	ARG	B	916	10.318	31.510	40.144	1.00	39.61	B	C
ATOM	3137	CB	ARG	B	916	10.593	30.538	39.001	1.00	41.84	B	C
ATOM	3138	CG	ARG	B	916	12.058	30.148	38.868	1.00	46.16	B	C
ATOM	3139	CD	ARG	B	916	12.473	29.106	39.908	1.00	51.32	B	C
ATOM	3140	NE	ARG	B	916	12.152	27.738	39.487	1.00	55.40	B	N
ATOM	3141	CZ	ARG	B	916	12.816	27.058	38.554	1.00	55.68	B	C
ATOM	3142	NH1	ARG	B	916	13.853	27.607	37.931	1.00	55.82	B	N
ATOM	3143	NH2	ARG	B	916	12.441	25.824	38.243	1.00	56.52	B	N
ATOM	3144	C	ARG	B	916	11.420	32.568	40.162	1.00	41.25	B	C

TABLE 2-continued

ATOM	3145	O	ARG	B	916	12.159	32.697	41.136	1.00	43.76	B	O
ATOM	3146	N	HIS	B	917	11.532	33.323	39.076	1.00	41.99	B	N
ATOM	3147	CA	HIS	B	917	12.578	34.324	38.954	1.00	41.77	B	C
ATOM	3148	CB	HIS	B	917	13.046	34.404	37.504	1.00	42.37	B	C
ATOM	3149	CG	HIS	B	917	13.113	33.077	36.817	1.00	43.07	B	C
ATOM	3150	CD2	HIS	B	917	14.170	32.340	36.402	1.00	43.65	B	C
ATOM	3151	ND1	HIS	B	917	11.987	32.376	36.443	1.00	44.34	B	N
ATOM	3152	CE1	HIS	B	917	12.347	31.267	35.822	1.00	44.79	B	C
ATOM	3153	NE2	HIS	B	917	13.666	31.222	35.783	1.00	44.29	B	N
ATOM	3154	C	HIS	B	917	12.179	35.707	39.419	1.00	41.88	B	C
ATOM	3155	O	HIS	B	917	12.767	36.696	38.989	1.00	41.51	B	O
ATOM	3156	N	ARG	B	918	11.184	35.778	40.294	1.00	42.86	B	N
ATOM	3157	CA	ARG	B	918	10.718	37.060	40.813	1.00	44.49	B	C
ATOM	3158	CB	ARG	B	918	9.802	36.849	42.017	1.00	45.42	B	C
ATOM	3159	CG	ARG	B	918	9.269	38.145	42.613	1.00	47.61	B	C
ATOM	3160	CD	ARG	B	918	8.412	37.874	43.839	1.00	49.68	B	C
ATOM	3161	NE	ARG	B	918	7.700	39.061	44.301	1.00	52.10	B	N
ATOM	3162	CZ	ARG	B	918	8.266	40.249	44.470	1.00	55.07	B	C
ATOM	3163	NH1	ARG	B	918	9.557	40.410	44.208	1.00	56.53	B	N
ATOM	3164	NH2	ARG	B	918	7.547	41.274	44.919	1.00	55.39	B	N
ATOM	3165	C	ARG	B	918	11.901	37.900	41.254	1.00	45.45	B	C
ATOM	3166	O	ARG	B	918	11.879	39.126	41.168	1.00	45.70	B	O
ATOM	3167	N	ALA	B	919	12.934	37.217	41.730	1.00	46.64	B	N
ATOM	3168	CA	ALA	B	919	14.135	37.868	42.219	1.00	46.70	B	C
ATOM	3169	CB	ALA	B	919	15.139	36.816	42.670	1.00	46.55	B	C
ATOM	3170	C	ALA	B	919	14.789	38.813	41.222	1.00	46.47	B	C
ATOM	3171	O	ALA	B	919	15.070	39.959	41.555	1.00	46.26	B	O
ATOM	3172	N	ARG	B	920	15.020	38.345	40.000	1.00	45.92	B	N
ATOM	3173	CA	ARG	B	920	15.680	39.180	39.011	1.00	46.71	B	C
ATOM	3174	CB	ARG	B	920	16.943	38.464	38.500	1.00	48.83	B	C
ATOM	3175	CG	ARG	B	920	16.764	36.992	38.107	1.00	50.57	B	C
ATOM	3176	CD	ARG	B	920	16.469	36.813	36.607	1.00	53.25	B	C
ATOM	3177	NE	ARG	B	920	16.442	35.401	36.206	1.00	54.08	B	N
ATOM	3178	CZ	ARG	B	920	16.323	34.966	34.952	1.00	52.53	B	C
ATOM	3179	NH1	ARG	B	920	16.216	35.828	33.945	1.00	51.03	B	N
ATOM	3180	NH2	ARG	B	920	16.317	33.664	34.707	1.00	50.11	B	N
ATOM	3181	C	ARG	B	920	14.833	39.657	37.839	1.00	45.45	B	C
ATOM	3182	O	ARG	B	920	15.245	39.558	36.688	1.00	44.69	B	O
ATOM	3183	N	LEU	B	921	13.659	40.204	38.138	1.00	45.01	B	N
ATOM	3184	CA	LEU	B	921	12.759	40.714	37.102	1.00	44.34	B	C
ATOM	3185	CB	LEU	B	921	11.623	39.720	36.840	1.00	44.36	B	C
ATOM	3186	CG	LEU	B	921	11.900	38.396	36.128	1.00	44.22	B	C
ATOM	3187	CD1	LEU	B	921	10.599	37.620	35.958	1.00	44.74	B	C
ATOM	3188	CD2	LEU	B	921	12.511	38.669	34.775	1.00	45.69	B	C
ATOM	3189	C	LEU	B	921	12.167	42.055	37.539	1.00	43.53	B	C
ATOM	3190	O	LEU	B	921	11.150	42.097	38.237	1.00	44.06	B	O
ATOM	3191	N	ASP	B	922	12.799	43.147	37.120	1.00	42.34	B	N
ATOM	3192	CA	ASP	B	922	12.335	44.477	37.499	1.00	41.85	B	C
ATOM	3193	CB	ASP	B	922	13.462	45.511	37.339	1.00	41.06	B	C
ATOM	3194	CG	ASP	B	922	13.976	45.614	35.909	1.00	42.29	B	C
ATOM	3195	OD1	ASP	B	922	13.142	45.659	34.975	1.00	39.58	B	O
ATOM	3196	OD2	ASP	B	922	15.219	45.666	35.730	1.00	43.31	B	O
ATOM	3197	C	ASP	B	922	11.106	44.943	36.731	1.00	39.87	B	C
ATOM	3198	O	ASP	B	922	10.672	44.306	35.781	1.00	41.23	B	O
ATOM	3199	N	ALA	B	923	10.552	46.068	37.158	1.00	37.59	B	N
ATOM	3200	CA	ALA	B	923	9.376	46.629	36.523	1.00	36.35	B	C
ATOM	3201	CB	ALA	B	923	9.017	47.950	37.187	1.00	35.54	B	C
ATOM	3202	C	ALA	B	923	9.553	46.824	35.017	1.00	35.68	B	C
ATOM	3203	O	ALA	B	923	8.588	46.730	34.260	1.00	35.30	B	O
ATOM	3204	N	SER	B	924	10.775	47.097	34.574	1.00	33.91	B	N
ATOM	3205	CA	SER	B	924	10.991	47.290	33.151	1.00	33.74	B	C
ATOM	3206	CB	SER	B	924	12.465	47.551	32.859	1.00	34.61	B	C
ATOM	3207	OG	SER	B	924	12.840	48.836	33.318	1.00	40.21	B	O
ATOM	3208	C	SER	B	924	10.523	46.061	32.390	1.00	33.14	B	C
ATOM	3209	O	SER	B	924	9.803	46.163	31.395	1.00	32.57	B	O
ATOM	3210	N	ARG	B	925	10.931	44.899	32.876	1.00	30.83	B	N
ATOM	3211	CA	ARG	B	925	10.552	43.653	32.259	1.00	31.63	B	C
ATOM	3212	CB	ARG	B	925	11.199	42.489	33.003	1.00	33.57	B	C
ATOM	3213	CG	ARG	B	925	10.900	41.147	32.394	1.00	35.20	B	C
ATOM	3214	CD	ARG	B	925	12.156	40.548	31.836	1.00	39.12	B	C
ATOM	3215	NE	ARG	B	925	12.823	41.461	30.920	1.00	41.44	B	N
ATOM	3216	CZ	ARG	B	925	14.029	41.240	30.416	1.00	42.69	B	C
ATOM	3217	NH1	ARG	B	925	14.576	42.117	29.585	1.00	43.07	B	N
ATOM	3218	NH2	ARG	B	925	14.685	40.138	30.753	1.00	41.67	B	N
ATOM	3219	C	ARG	B	925	9.035	43.493	32.286	1.00	31.85	B	C
ATOM	3220	O	ARG	B	925	8.415	43.165	31.270	1.00	30.05	B	O
ATOM	3221	N	LEU	B	926	8.442	43.723	33.457	1.00	30.42	B	N
ATOM	3222	CA	LEU	B	926	6.998	43.589	33.614	1.00	28.04	B	C
ATOM	3223	CB	LEU	B	926	6.570	44.056	35.002	1.00	27.26	B	C
ATOM	3224	CG	LEU	B	926	7.230	43.348	36.185	1.00	28.68	B	C

TABLE 2-continued

ATOM	3225	CD1	LEU	B	926	6.539	43.811	37.487	1.00	26.24	B	C
ATOM	3226	CD2	LEU	B	926	7.119	41.819	36.004	1.00	24.28	B	C
ATOM	3227	C	LEU	B	926	6.285	44.412	32.551	1.00	27.32	B	C
ATOM	3228	O	LEU	B	926	5.294	43.971	31.969	1.00	27.38	B	O
ATOM	3229	N	LEU	B	927	6.806	45.610	32.302	1.00	25.79	B	N
ATOM	3230	CA	LEU	B	927	6.239	46.509	31.305	1.00	25.06	B	C
ATOM	3231	CB	LEU	B	927	6.829	47.921	31.474	1.00	22.03	B	C
ATOM	3232	CG	LEU	B	927	6.221	48.706	32.650	1.00	20.16	B	C
ATOM	3233	CD1	LEU	B	927	6.929	50.021	32.861	1.00	19.40	B	C
ATOM	3234	CD2	LEU	B	927	4.742	48.949	32.363	1.00	21.09	B	C
ATOM	3235	C	LEU	B	927	6.488	45.959	29.897	1.00	25.65	B	C
ATOM	3236	O	LEU	B	927	5.660	46.115	28.996	1.00	25.31	B	O
ATOM	3237	N	LEU	B	928	7.622	45.298	29.714	1.00	26.41	B	N
ATOM	3238	CA	LEU	B	928	7.922	44.693	28.429	1.00	27.69	B	C
ATOM	3239	CB	LEU	B	928	9.310	44.038	28.452	1.00	27.36	B	C
ATOM	3240	CG	LEU	B	928	9.829	43.541	27.093	1.00	29.18	B	C
ATOM	3241	CD1	LEU	B	928	9.870	44.697	26.100	1.00	26.86	B	C
ATOM	3242	CD2	LEU	B	928	11.220	42.930	27.259	1.00	28.41	B	C
ATOM	3243	C	LEU	B	928	6.840	43.635	28.141	1.00	27.69	B	C
ATOM	3244	O	LEU	B	928	6.178	43.695	27.109	1.00	29.81	B	O
ATOM	3245	N	TYR	B	929	6.649	42.685	29.059	1.00	26.62	B	N
ATOM	3246	CA	TYR	B	929	5.646	41.634	28.873	1.00	25.73	B	C
ATOM	3247	CB	TYR	B	929	5.570	40.676	30.078	1.00	24.73	B	C
ATOM	3248	CG	TYR	B	929	6.863	39.964	30.423	1.00	25.65	B	C
ATOM	3249	CD1	TYR	B	929	7.710	39.488	29.428	1.00	26.25	B	C
ATOM	3250	CE1	TYR	B	929	8.900	38.847	29.749	1.00	26.35	B	C
ATOM	3251	CD2	TYR	B	929	7.241	39.771	31.750	1.00	25.40	B	C
ATOM	3252	CE2	TYR	B	929	8.421	39.131	32.077	1.00	23.77	B	C
ATOM	3253	CZ	TYR	B	929	9.245	38.675	31.077	1.00	26.10	B	C
ATOM	3254	OH	TYR	B	929	10.427	38.057	31.394	1.00	26.76	B	O
ATOM	3255	C	TYR	B	929	4.270	42.236	28.676	1.00	24.74	B	C
ATOM	3256	O	TYR	B	929	3.439	41.656	27.995	1.00	23.60	B	O
ATOM	3257	N	SER	B	930	4.029	43.391	29.289	1.00	25.64	B	N
ATOM	3258	CA	SER	B	930	2.730	44.052	29.183	1.00	26.06	B	C
ATOM	3259	CB	SER	B	930	2.622	45.176	30.213	1.00	26.82	B	C
ATOM	3260	OG	SER	B	930	2.832	44.674	31.525	1.00	28.96	B	O
ATOM	3261	C	SER	B	930	2.512	44.600	27.782	1.00	25.97	B	C
ATOM	3262	O	SER	B	930	1.434	44.454	27.210	1.00	26.37	B	O
ATOM	3263	N	SER	B	931	3.550	45.208	27.221	1.00	26.24	B	N
ATOM	3264	CA	SER	B	931	3.472	45.768	25.877	1.00	24.72	B	C
ATOM	3265	CB	SER	B	931	4.746	46.562	25.559	1.00	25.41	B	C
ATOM	3266	OG	SER	B	931	4.663	47.190	24.288	1.00	25.63	B	O
ATOM	3267	C	SER	B	931	3.272	44.671	24.829	1.00	22.71	B	C
ATOM	3268	O	SER	B	931	2.440	44.804	23.937	1.00	22.21	B	O
ATOM	3269	N	GLN	B	932	4.043	43.594	24.926	1.00	21.13	B	N
ATOM	3270	CA	GLN	B	932	3.922	42.501	23.967	1.00	20.19	B	C
ATOM	3271	CB	GLN	B	932	5.018	41.469	24.195	1.00	18.59	B	C
ATOM	3272	CG	GLN	B	932	6.417	42.034	24.201	1.00	16.41	B	C
ATOM	3273	CD	GLN	B	932	7.450	40.960	24.447	1.00	18.92	B	C
ATOM	3274	OE1	GLN	B	932	7.173	39.963	25.111	1.00	19.34	B	O
ATOM	3275	NE2	GLN	B	932	8.659	41.161	23.928	1.00	20.97	B	N
ATOM	3276	C	GLN	B	932	2.552	41.830	24.062	1.00	20.13	B	C
ATOM	3277	O	GLN	B	932	1.987	41.438	23.052	1.00	20.51	B	O
ATOM	3278	N	ILE	B	933	2.014	41.708	25.272	1.00	19.68	B	N
ATOM	3279	CA	ILE	B	933	0.714	41.087	25.452	1.00	20.83	B	C
ATOM	3280	CB	ILE	B	933	0.396	40.865	26.957	1.00	20.65	B	C
ATOM	3281	CG2	ILE	B	933	−1.099	40.537	27.156	1.00	18.30	B	C
ATOM	3282	CG1	ILE	B	933	1.274	39.731	27.506	1.00	17.48	B	C
ATOM	3283	CD1	ILE	B	933	1.297	39.640	29.005	1.00	14.75	B	C
ATOM	3284	C	ILE	B	933	−0.330	41.997	24.825	1.00	23.98	B	C
ATOM	3285	O	ILE	B	933	−1.262	41.530	24.165	1.00	27.92	B	O
ATOM	3286	N	CYS	B	934	−0.162	43.302	25.009	1.00	24.95	B	N
ATOM	3287	CA	CYS	B	934	−1.096	44.271	24.450	1.00	23.96	B	C
ATOM	3288	CB	CYS	B	934	−0.771	45.675	24.962	1.00	22.48	B	C
ATOM	3289	SG	CYS	B	934	−2.047	46.909	24.612	1.00	26.90	B	S
ATOM	3290	C	CYS	B	934	−1.027	44.258	22.927	1.00	23.61	B	C
ATOM	3291	O	CYS	B	934	−2.050	44.291	22.236	1.00	21.24	B	O
ATOM	3292	N	LYS	B	935	0.189	44.212	22.401	1.00	25.11	B	N
ATOM	3293	CA	LYS	B	935	0.378	44.212	20.957	1.00	25.85	B	C
ATOM	3294	CB	LYS	B	935	1.878	44.169	20.629	1.00	28.60	B	C
ATOM	3295	CG	LYS	B	935	2.217	44.378	19.162	1.00	31.12	B	C
ATOM	3296	CD	LYS	B	935	1.628	45.673	18.661	1.00	36.08	B	C
ATOM	3297	CE	LYS	B	935	1.778	45.817	17.159	1.00	37.38	B	C
ATOM	3298	NZ	LYS	B	935	0.958	46.965	16.669	1.00	39.57	B	N
ATOM	3299	C	LYS	B	935	−0.356	43.008	20.370	1.00	25.95	B	C
ATOM	3300	O	LYS	B	935	−1.099	43.147	19.403	1.00	26.64	B	O
ATOM	3301	N	GLY	B	936	−0.176	41.840	20.981	1.00	24.87	B	N
ATOM	3302	CA	GLY	B	936	−0.846	40.645	20.503	1.00	25.53	B	C
ATOM	3303	C	GLY	B	936	−2.367	40.737	20.520	1.00	25.87	B	C
ATOM	3304	O	GLY	B	936	−3.046	40.382	19.541	1.00	22.39	B	O

TABLE 2-continued

ATOM	3305	N	MET	B	937	−2.903	41.218	21.637	1.00	24.22	B	N
ATOM	3306	CA	MET	B	937	−4.344	41.354	21.784	1.00	25.26	B	C
ATOM	3307	CB	MET	B	937	−4.680	41.810	23.208	1.00	22.36	B	C
ATOM	3308	CG	MET	B	937	−4.476	40.693	24.213	1.00	23.06	B	C
ATOM	3309	SD	MET	B	937	−5.425	39.200	23.698	1.00	20.48	B	S
ATOM	3310	CE	MET	B	937	−7.049	39.901	23.661	1.00	15.72	B	C
ATOM	3311	C	MET	B	937	−4.908	42.319	20.746	1.00	25.24	B	C
ATOM	3312	O	MET	B	937	−6.030	42.155	20.276	1.00	25.83	B	O
ATOM	3313	N	GLU	B	938	−4.115	43.314	20.372	1.00	27.10	B	N
ATOM	3314	CA	GLU	B	938	−4.553	44.279	19.373	1.00	29.62	B	C
ATOM	3315	CB	GLU	B	938	−3.575	45.458	19.307	1.00	30.48	B	C
ATOM	3316	CG	GLU	B	938	−3.911	46.454	18.221	1.00	35.52	B	C
ATOM	3317	CD	GLU	B	938	−2.834	47.506	18.000	1.00	38.79	B	C
ATOM	3318	OE1	GLU	B	938	−1.636	47.140	17.896	1.00	40.52	B	O
ATOM	3319	OE2	GLU	B	938	−3.198	48.698	17.915	1.00	38.59	B	O
ATOM	3320	C	GLU	B	938	−4.675	43.609	17.993	1.00	28.94	B	C
ATOM	3321	O	GLU	B	938	−5.659	43.803	17.282	1.00	27.75	B	O
ATOM	3322	N	TYR	B	939	−3.677	42.819	17.623	1.00	27.57	B	N
ATOM	3323	CA	TYR	B	939	−3.720	42.139	16.345	1.00	27.18	B	C
ATOM	3324	CB	TYR	B	939	−2.428	41.354	16.133	1.00	26.82	B	C
ATOM	3325	CG	TYR	B	939	−2.512	40.410	14.969	1.00	28.23	B	C
ATOM	3326	CD1	TYR	B	939	−2.672	40.879	13.676	1.00	27.67	B	C
ATOM	3327	CE1	TYR	B	939	−2.818	39.995	12.613	1.00	27.50	B	C
ATOM	3328	CD2	TYR	B	939	−2.495	39.034	15.170	1.00	30.11	B	C
ATOM	3329	CE2	TYR	B	939	−2.641	38.143	14.113	1.00	27.69	B	C
ATOM	3330	CZ	TYR	B	939	−2.803	38.630	12.844	1.00	25.76	B	C
ATOM	3331	OH	TYR	B	939	−2.969	37.746	11.809	1.00	28.05	B	O
ATOM	3332	C	TYR	B	939	−4.936	41.196	16.283	1.00	27.22	B	C
ATOM	3333	O	TYR	B	939	−5.730	41.229	15.333	1.00	25.58	B	O
ATOM	3334	N	LEU	B	940	−5.084	40.365	17.312	1.00	27.83	B	N
ATOM	3335	CA	LEU	B	940	−6.194	39.422	17.370	1.00	27.45	B	C
ATOM	3336	CB	LEU	B	940	−6.159	38.621	18.678	1.00	25.08	B	C
ATOM	3337	CG	LEU	B	940	−4.922	37.722	18.864	1.00	27.64	B	C
ATOM	3338	CD1	LEU	B	940	−5.154	36.762	20.017	1.00	24.40	B	C
ATOM	3339	CD2	LEU	B	940	−4.625	36.931	17.591	1.00	27.99	B	C
ATOM	3340	C	LEU	B	940	−7.533	40.138	17.216	1.00	26.86	B	C
ATOM	3341	O	LEU	B	940	−8.439	39.627	16.562	1.00	28.15	B	O
ATOM	3342	N	GLY	B	941	−7.643	41.329	17.796	1.00	26.05	B	N
ATOM	3343	CA	GLY	B	941	−8.879	42.092	17.707	1.00	23.74	B	C
ATOM	3344	C	GLY	B	941	−9.205	42.585	16.312	1.00	21.83	B	C
ATOM	3345	O	GLY	B	941	−10.338	42.461	15.841	1.00	19.35	B	O
ATOM	3346	N	SER	B	942	−8.206	43.153	15.651	1.00	21.40	B	N
ATOM	3347	CA	SER	B	942	−8.384	43.660	14.307	1.00	23.07	B	C
ATOM	3348	CB	SER	B	942	−7.086	44.309	13.815	1.00	20.62	B	C
ATOM	3349	OG	SER	B	942	−6.006	43.388	13.817	1.00	16.12	B	O
ATOM	3350	C	SER	B	942	−8.801	42.536	13.359	1.00	26.33	B	C
ATOM	3351	O	SER	B	942	−9.307	42.793	12.260	1.00	29.50	B	O
ATOM	3352	N	ARG	B	943	−8.593	41.293	13.782	1.00	24.35	B	N
ATOM	3353	CA	ARG	B	943	−8.954	40.161	12.963	1.00	23.61	B	C
ATOM	3354	CB	ARG	B	943	−7.827	39.141	12.956	1.00	26.33	B	C
ATOM	3355	CG	ARG	B	943	−6.624	39.601	12.198	1.00	29.12	B	C
ATOM	3356	CD	ARG	B	943	−6.909	39.625	10.718	1.00	34.41	B	C
ATOM	3357	NE	ARG	B	943	−5.854	40.306	9.975	1.00	37.63	B	N
ATOM	3358	CZ	ARG	B	943	−5.479	41.557	10.216	1.00	38.64	B	C
ATOM	3359	NH1	ARG	B	943	−4.512	42.127	9.502	1.00	38.73	B	N
ATOM	3360	NH2	ARG	B	943	−6.075	42.233	11.188	1.00	40.59	B	N
ATOM	3361	C	ARG	B	943	−10.221	39.535	13.494	1.00	24.10	B	C
ATOM	3362	O	ARG	B	943	−10.549	38.392	13.171	1.00	23.79	B	O
ATOM	3363	N	ARG	B	944	−10.929	40.288	14.327	1.00	25.80	B	N
ATOM	3364	CA	ARG	B	944	−12.190	39.832	14.902	1.00	27.06	B	C
ATOM	3365	CB	ARG	B	944	−13.222	39.690	13.786	1.00	29.29	B	C
ATOM	3366	CG	ARG	B	944	−13.328	40.944	12.931	1.00	33.03	B	C
ATOM	3367	CD	ARG	B	944	−14.432	40.833	11.901	1.00	37.88	B	C
ATOM	3368	NE	ARG	B	944	−14.475	42.000	11.018	1.00	41.34	B	N
ATOM	3369	CZ	ARG	B	944	−14.967	43.192	11.345	1.00	42.38	B	C
ATOM	3370	NH1	ARG	B	944	−15.482	43.410	12.550	1.00	43.09	B	N
ATOM	3371	NH2	ARG	B	944	−14.928	44.179	10.460	1.00	43.07	B	N
ATOM	3372	C	ARG	B	944	−12.137	38.538	15.722	1.00	27.11	B	C
ATOM	3373	O	ARG	B	944	−13.102	37.777	15.739	1.00	27.61	B	O
ATOM	3374	N	CYS	B	945	−11.020	38.298	16.404	1.00	24.94	B	N
ATOM	3375	CA	CYS	B	945	−10.863	37.112	17.239	1.00	24.53	B	C
ATOM	3376	CB	CYS	B	945	−9.489	36.485	17.004	1.00	25.33	B	C
ATOM	3377	SG	CYS	B	945	−9.124	35.025	18.022	1.00	30.16	B	S
ATOM	3378	C	CYS	B	945	−11.014	37.466	18.728	1.00	23.62	B	C
ATOM	3379	O	CYS	B	945	−10.477	38.472	19.188	1.00	23.54	B	O
ATOM	3380	N	VAL	B	946	−11.745	36.635	19.468	1.00	22.35	B	N
ATOM	3381	CA	VAL	B	946	−11.959	36.844	20.900	1.00	21.99	B	C
ATOM	3382	CB	VAL	B	946	−13.468	36.922	21.219	1.00	19.57	B	C
ATOM	3383	CG1	VAL	B	946	−13.699	37.058	22.729	1.00	17.37	B	C
ATOM	3384	CG2	VAL	B	946	−14.064	38.114	20.500	1.00	17.89	B	C

TABLE 2-continued

ATOM	3385	C	VAL	B	946	−11.300	35.725	21.728	1.00	23.03	B	C
ATOM	3386	O	VAL	B	946	−11.554	34.537	21.510	1.00	26.36	B	O
ATOM	3387	N	HIS	B	947	−10.454	36.120	22.671	1.00	20.78	B	N
ATOM	3388	CA	HIS	B	947	−9.731	35.172	23.510	1.00	22.55	B	C
ATOM	3389	CB	HIS	B	947	−8.707	35.896	24.395	1.00	20.18	B	C
ATOM	3390	CG	HIS	B	947	−7.680	34.980	24.980	1.00	17.97	B	C
ATOM	3391	CD2	HIS	B	947	−7.802	33.946	25.842	1.00	16.23	B	C
ATOM	3392	ND1	HIS	B	947	−6.363	34.987	24.573	1.00	16.76	B	N
ATOM	3393	CE1	HIS	B	947	−5.719	33.990	25.152	1.00	14.12	B	C
ATOM	3394	NE2	HIS	B	947	−6.569	33.341	25.925	1.00	16.69	B	N
ATOM	3395	C	HIS	B	947	−10.636	34.354	24.404	1.00	22.03	B	C
ATOM	3396	O	HIS	B	947	−10.644	33.138	24.324	1.00	24.74	B	O
ATOM	3397	N	ARG	B	948	−11.378	35.030	25.268	1.00	24.81	B	N
ATOM	3398	CA	ARG	B	948	−12.302	34.386	26.204	1.00	29.26	B	C
ATOM	3399	CB	ARG	B	948	−13.059	33.233	25.530	1.00	32.27	B	C
ATOM	3400	CG	ARG	B	948	−14.516	33.556	25.207	1.00	37.63	B	C
ATOM	3401	CD	ARG	B	948	−15.406	32.314	25.302	1.00	43.26	B	C
ATOM	3402	NE	ARG	B	948	−15.330	31.674	26.617	1.00	46.10	B	N
ATOM	3403	CZ	ARG	B	948	−16.182	30.753	27.057	1.00	48.54	B	C
ATOM	3404	NH1	ARG	B	948	−16.021	30.238	28.268	1.00	49.33	B	N
ATOM	3405	NH2	ARG	B	948	−17.195	30.352	26.294	1.00	49.77	B	N
ATOM	3406	C	ARG	B	948	−11.697	33.889	27.522	1.00	28.75	B	C
ATOM	3407	O	ARG	B	948	−12.397	33.831	28.532	1.00	30.89	B	O
ATOM	3408	N	ASP	B	949	−10.415	33.542	27.536	1.00	28.05	B	N
ATOM	3409	CA	ASP	B	949	−9.801	33.070	28.773	1.00	26.91	B	C
ATOM	3410	CB	ASP	B	949	−9.766	31.535	28.779	1.00	28.13	B	C
ATOM	3411	CG	ASP	B	949	−9.324	30.955	30.116	1.00	30.51	B	C
ATOM	3412	OD1	ASP	B	949	−9.744	31.469	31.166	1.00	32.59	B	O
ATOM	3413	OD2	ASP	B	949	−8.565	29.969	30.124	1.00	31.18	B	O
ATOM	3414	C	ASP	B	949	−8.393	33.653	28.937	1.00	25.45	B	C
ATOM	3415	O	ASP	B	949	−7.426	32.927	29.151	1.00	25.26	B	O
ATOM	3416	N	LEU	B	950	−8.279	34.971	28.829	1.00	23.58	B	N
ATOM	3417	CA	LEU	B	950	−6.976	35.608	28.958	1.00	22.80	B	C
ATOM	3418	CB	LEU	B	950	−7.000	37.024	28.392	1.00	20.62	B	C
ATOM	3419	CG	LEU	B	950	−5.676	37.798	28.285	1.00	18.98	B	C
ATOM	3420	CD1	LEU	B	950	−4.751	37.141	27.253	1.00	13.37	B	C
ATOM	3421	CD2	LEU	B	950	−5.970	39.246	27.867	1.00	12.59	B	C
ATOM	3422	C	LEU	B	950	−6.618	35.644	30.425	1.00	22.41	B	C
ATOM	3423	O	LEU	B	950	−7.473	35.910	31.264	1.00	20.85	B	O
ATOM	3424	N	ALA	B	951	−5.352	35.362	30.717	1.00	20.76	B	N
ATOM	3425	CA	ALA	B	951	−4.852	35.331	32.078	1.00	17.81	B	C
ATOM	3426	CB	ALA	B	951	−5.594	34.306	32.859	1.00	12.31	B	C
ATOM	3427	C	ALA	B	951	−3.368	34.997	32.041	1.00	19.23	B	C
ATOM	3428	O	ALA	B	951	−2.879	34.395	31.084	1.00	22.05	B	O
ATOM	3429	N	ALA	B	952	−2.647	35.393	33.083	1.00	19.76	B	N
ATOM	3430	CA	ALA	B	952	−1.209	35.154	33.157	1.00	18.16	B	C
ATOM	3431	CB	ALA	B	952	−0.671	35.622	34.518	1.00	18.36	B	C
ATOM	3432	C	ALA	B	952	−0.831	33.696	32.911	1.00	17.28	B	C
ATOM	3433	O	ALA	B	952	0.298	33.403	32.503	1.00	18.38	B	O
ATOM	3434	N	ARG	B	953	−1.761	32.783	33.174	1.00	17.20	B	N
ATOM	3435	CA	ARG	B	953	−1.501	31.359	32.958	1.00	19.59	B	C
ATOM	3436	CB	ARG	B	953	−2.502	30.490	33.734	1.00	18.77	B	C
ATOM	3437	CG	ARG	B	953	−3.902	30.571	33.184	1.00	18.10	B	C
ATOM	3438	CD	ARG	B	953	−4.843	29.692	33.962	1.00	19.26	B	C
ATOM	3439	NE	ARG	B	953	−6.241	30.056	33.733	1.00	19.94	B	N
ATOM	3440	CZ	ARG	B	953	−6.897	30.984	34.421	1.00	20.48	B	C
ATOM	3441	NH1	ARG	B	953	−6.292	31.652	35.395	1.00	22.23	B	N
ATOM	3442	NH2	ARG	B	953	−8.161	31.246	34.137	1.00	19.77	B	N
ATOM	3443	C	ARG	B	953	−1.606	31.044	31.462	1.00	21.37	B	C
ATOM	3444	O	ARG	B	953	−0.991	30.090	30.967	1.00	20.33	B	O
ATOM	3445	N	ASN	B	954	−2.389	31.837	30.734	1.00	21.32	B	N
ATOM	3446	CA	ASN	B	954	−2.507	31.594	29.301	1.00	22.57	B	C
ATOM	3447	CB	ASN	B	954	−3.966	31.740	28.836	1.00	19.78	B	C
ATOM	3448	CG	ASN	B	954	−4.824	30.542	29.243	1.00	18.80	B	C
ATOM	3449	OD1	ASN	B	954	−4.347	29.404	29.258	1.00	16.51	B	O
ATOM	3450	ND2	ASN	B	954	−6.088	30.791	29.568	1.00	18.61	B	N
ATOM	3451	C	ASN	B	954	−1.563	32.460	28.467	1.00	23.15	B	C
ATOM	3452	O	ASN	B	954	−1.837	32.764	27.305	1.00	24.11	B	O
ATOM	3453	N	ILE	B	955	−0.447	32.840	29.085	1.00	22.78	B	N
ATOM	3454	CA	ILE	B	955	0.600	33.636	28.446	1.00	23.25	B	C
ATOM	3455	CB	ILE	B	955	0.911	34.930	29.252	1.00	22.42	B	C
ATOM	3456	CG2	ILE	B	955	2.137	35.627	28.660	1.00	21.63	B	C
ATOM	3457	CG1	ILE	B	955	−0.317	35.851	29.285	1.00	20.99	B	C
ATOM	3458	CD1	ILE	B	955	−0.663	36.492	27.966	1.00	19.44	B	C
ATOM	3459	C	ILE	B	955	1.846	32.761	28.489	1.00	24.65	B	C
ATOM	3460	O	ILE	B	955	2.390	32.527	29.570	1.00	27.02	B	O
ATOM	3461	N	LEU	B	956	2.302	32.274	27.339	1.00	24.24	B	N
ATOM	3462	CA	LEU	B	956	3.480	31.405	27.315	1.00	24.52	B	C
ATOM	3463	CB	LEU	B	956	3.298	30.311	26.244	1.00	23.14	B	C
ATOM	3464	CG	LEU	B	956	2.291	29.206	26.637	1.00	21.34	B	C

TABLE 2-continued

ATOM	3465	CD1	LEU	B	956	1.936	28.336	25.446	1.00	20.11	B	C
ATOM	3466	CD2	LEU	B	956	2.875	28.338	27.737	1.00	19.45	B	C
ATOM	3467	C	LEU	B	956	4.793	32.169	27.113	1.00	26.13	B	C
ATOM	3468	O	LEU	B	956	4.827	33.196	26.437	1.00	27.09	B	O
ATOM	3469	N	VAL	B	957	5.869	31.664	27.716	1.00	26.24	B	N
ATOM	3470	CA	VAL	B	957	7.187	32.296	27.631	1.00	25.04	B	C
ATOM	3471	CB	VAL	B	957	8.000	32.098	28.950	1.00	25.69	B	C
ATOM	3472	CG1	VAL	B	957	9.431	32.628	28.780	1.00	21.14	B	C
ATOM	3473	CG2	VAL	B	957	7.297	32.805	30.113	1.00	24.99	B	C
ATOM	3474	C	VAL	B	957	8.045	31.787	26.477	1.00	25.81	B	C
ATOM	3475	O	VAL	B	957	8.475	30.630	26.469	1.00	27.02	B	O
ATOM	3476	N	GLU	B	958	8.288	32.649	25.498	1.00	26.44	B	N
ATOM	3477	CA	GLU	B	958	9.126	32.274	24.368	1.00	28.76	B	C
ATOM	3478	CB	GLU	B	958	8.912	33.237	23.196	1.00	28.56	B	C
ATOM	3479	CG	GLU	B	958	9.876	33.025	22.035	1.00	30.73	B	C
ATOM	3480	CD	GLU	B	958	9.599	31.765	21.224	1.00	32.95	B	C
ATOM	3481	OE1	GLU	B	958	10.401	31.465	20.315	1.00	35.94	B	O
ATOM	3482	OE2	GLU	B	958	8.592	31.075	21.474	1.00	33.94	B	O
ATOM	3483	C	GLU	B	958	10.567	32.364	24.868	1.00	29.72	B	C
ATOM	3484	O	GLU	B	958	11.401	31.514	24.571	1.00	30.94	B	O
ATOM	3485	N	SER	B	959	10.842	33.404	25.645	1.00	31.11	B	N
ATOM	3486	CA	SER	B	959	12.164	33.609	26.210	1.00	32.58	B	C
ATOM	3487	CB	SER	B	959	13.152	34.054	25.137	1.00	30.97	B	C
ATOM	3488	OG	SER	B	959	13.235	35.465	25.113	1.00	33.82	B	O
ATOM	3489	C	SER	B	959	12.039	34.688	27.286	1.00	34.54	B	C
ATOM	3490	O	SER	B	959	10.961	35.246	27.482	1.00	33.70	B	O
ATOM	3491	N	GLU	B	960	13.147	34.978	27.962	1.00	35.55	B	N
ATOM	3492	CA	GLU	B	960	13.189	35.961	29.038	1.00	36.85	B	C
ATOM	3493	CB	GLU	B	960	14.615	36.058	29.594	1.00	39.46	B	C
ATOM	3494	CG	GLU	B	960	15.207	34.704	29.961	1.00	46.26	B	C
ATOM	3495	CD	GLU	B	960	15.453	33.813	28.738	1.00	50.12	B	C
ATOM	3496	OE1	GLU	B	960	15.423	32.565	28.888	1.00	51.89	B	O
ATOM	3497	OE2	GLU	B	960	15.684	34.358	27.629	1.00	51.11	B	O
ATOM	3498	C	GLU	B	960	12.703	37.344	28.622	1.00	35.60	B	C
ATOM	3499	O	GLU	B	960	12.252	38.134	29.455	1.00	35.96	B	O
ATOM	3500	N	ALA	B	961	12.788	37.644	27.336	1.00	32.86	B	N
ATOM	3501	CA	ALA	B	961	12.347	38.945	26.869	1.00	31.54	B	C
ATOM	3502	CB	ALA	B	961	13.542	39.737	26.370	1.00	32.46	B	C
ATOM	3503	C	ALA	B	961	11.282	38.857	25.776	1.00	30.73	B	C
ATOM	3504	O	ALA	B	961	11.186	39.740	24.928	1.00	30.46	B	O
ATOM	3505	N	HIS	B	962	10.474	37.801	25.802	1.00	29.79	B	N
ATOM	3506	CA	HIS	B	962	9.433	37.627	24.791	1.00	28.25	B	C
ATOM	3507	CB	HIS	B	962	10.070	37.195	23.468	1.00	27.95	B	C
ATOM	3508	CG	HIS	B	962	9.109	37.137	22.322	1.00	28.31	B	C
ATOM	3509	CD2	HIS	B	962	7.810	36.764	22.263	1.00	28.79	B	C
ATOM	3510	ND1	HIS	B	962	9.461	37.504	21.041	1.00	31.00	B	N
ATOM	3511	CE1	HIS	B	962	8.418	37.365	20.243	1.00	29.74	B	C
ATOM	3512	NE2	HIS	B	962	7.404	36.918	20.959	1.00	30.22	B	N
ATOM	3513	C	HIS	B	962	8.354	36.623	25.191	1.00	28.20	B	C
ATOM	3514	O	HIS	B	962	8.611	35.419	25.293	1.00	28.83	B	O
ATOM	3515	N	VAL	B	963	7.139	37.123	25.393	1.00	25.95	B	N
ATOM	3516	CA	VAL	B	963	6.013	36.279	25.768	1.00	24.74	B	C
ATOM	3517	CB	VAL	B	963	5.334	36.815	27.055	1.00	23.78	B	C
ATOM	3518	CG1	VAL	B	963	6.308	36.684	28.219	1.00	21.06	B	C
ATOM	3519	CG2	VAL	B	963	4.897	38.280	26.876	1.00	17.99	B	C
ATOM	3520	C	VAL	B	963	4.980	36.159	24.644	1.00	25.21	B	C
ATOM	3521	O	VAL	B	963	4.918	37.004	23.754	1.00	26.73	B	O
ATOM	3522	N	LYS	B	964	4.176	35.102	24.683	1.00	24.96	B	N
ATOM	3523	CA	LYS	B	964	3.155	34.877	23.655	1.00	25.16	B	C
ATOM	3524	CB	LYS	B	964	3.553	33.727	22.729	1.00	25.01	B	C
ATOM	3525	CG	LYS	B	964	4.701	34.011	21.783	1.00	24.77	B	C
ATOM	3526	CD	LYS	B	964	5.061	32.737	21.023	1.00	26.76	B	C
ATOM	3527	CE	LYS	B	964	6.084	32.982	19.931	1.00	28.31	B	C
ATOM	3528	NZ	LYS	B	964	6.299	31.771	19.085	1.00	28.80	B	N
ATOM	3529	C	LYS	B	964	1.794	34.547	24.243	1.00	25.01	B	C
ATOM	3530	O	LYS	B	964	1.702	33.913	25.296	1.00	25.35	B	O
ATOM	3531	N	ILE	B	965	0.743	34.982	23.549	1.00	24.07	B	N
ATOM	3532	CA	ILE	B	965	−0.629	34.721	23.971	1.00	23.22	B	C
ATOM	3533	CB	ILE	B	965	−1.615	35.726	23.326	1.00	24.06	B	C
ATOM	3534	CG2	ILE	B	965	−3.035	35.382	23.708	1.00	22.79	B	C
ATOM	3535	CG1	ILE	B	965	−1.303	37.145	23.800	1.00	24.57	B	C
ATOM	3536	CD1	ILE	B	965	−2.055	38.217	23.050	1.00	24.62	B	C
ATOM	3537	C	ILE	B	965	−1.010	33.305	23.539	1.00	23.90	B	C
ATOM	3538	O	ILE	B	965	−0.729	32.883	22.406	1.00	23.98	B	O
ATOM	3539	N	ALA	B	966	−1.653	32.577	24.445	1.00	23.77	B	N
ATOM	3540	CA	ALA	B	966	−2.062	31.199	24.181	1.00	22.79	B	C
ATOM	3541	CB	ALA	B	966	−1.185	30.222	24.992	1.00	20.10	B	C
ATOM	3542	C	ALA	B	966	−3.529	30.935	24.494	1.00	21.11	B	C
ATOM	3543	O	ALA	B	966	−4.151	31.653	25.272	1.00	19.04	B	O
ATOM	3544	N	ASP	B	967	−4.065	29.887	23.875	1.00	20.78	B	N

TABLE 2-continued

ATOM	3545	CA	ASP	B	967	−5.440	29.482	24.089	1.00	22.00	B	C
ATOM	3546	CB	ASP	B	967	−5.625	29.127	25.555	1.00	24.96	B	C
ATOM	3547	CG	ASP	B	967	−5.199	27.729	25.851	1.00	28.88	B	C
ATOM	3548	OD1	ASP	B	967	−4.008	27.409	25.637	1.00	35.17	B	O
ATOM	3549	OD2	ASP	B	967	−6.058	26.943	26.279	1.00	30.71	B	O
ATOM	3550	C	ASP	B	967	−6.489	30.498	23.677	1.00	21.34	B	C
ATOM	3551	O	ASP	B	967	−7.487	30.687	24.374	1.00	19.28	B	O
ATOM	3552	N	PHE	B	968	−6.256	31.147	22.546	1.00	21.34	B	N
ATOM	3553	CA	PHE	B	968	−7.172	32.154	22.042	1.00	23.12	B	C
ATOM	3554	CB	PHE	B	968	−6.373	33.312	21.440	1.00	19.95	B	C
ATOM	3555	CG	PHE	B	968	−5.428	32.897	20.346	1.00	20.95	B	C
ATOM	3556	CD1	PHE	B	968	−5.844	32.850	19.021	1.00	19.89	B	C
ATOM	3557	CD2	PHE	B	968	−4.107	32.586	20.637	1.00	20.34	B	C
ATOM	3558	CE1	PHE	B	968	−4.955	32.507	18.000	1.00	19.70	B	C
ATOM	3559	CE2	PHE	B	968	−3.210	32.240	19.623	1.00	20.58	B	C
ATOM	3560	CZ	PHE	B	968	−3.633	32.202	18.304	1.00	20.85	B	C
ATOM	3561	C	PHE	B	968	−8.156	31.609	21.005	1.00	24.50	B	C
ATOM	3562	O	PHE	B	968	−7.913	30.571	20.384	1.00	24.19	B	O
ATOM	3563	N	GLY	B	969	−9.273	32.316	20.855	1.00	25.76	B	N
ATOM	3564	CA	GLY	B	969	−10.296	31.964	19.888	1.00	28.10	B	C
ATOM	3565	C	GLY	B	969	−10.837	30.551	19.900	1.00	28.39	B	C
ATOM	3566	O	GLY	B	969	−10.864	29.902	18.863	1.00	29.91	B	O
ATOM	3567	N	LEU	B	970	−11.287	30.083	21.060	1.00	29.33	B	N
ATOM	3568	CA	LEU	B	970	−11.832	28.733	21.198	1.00	27.90	B	C
ATOM	3569	CB	LEU	B	970	−11.023	27.938	22.221	1.00	25.43	B	C
ATOM	3570	CG	LEU	B	970	−10.135	26.800	21.722	1.00	27.12	B	C
ATOM	3571	CD1	LEU	B	970	−9.196	27.267	20.639	1.00	25.92	B	C
ATOM	3572	CD2	LEU	B	970	−9.351	26.256	22.897	1.00	30.60	B	C
ATOM	3573	C	LEU	B	970	−13.285	28.765	21.631	1.00	27.45	B	C
ATOM	3574	O	LEU	B	970	−13.894	27.714	21.823	1.00	28.00	B	O
ATOM	3575	N	ALA	B	971	−13.830	29.974	21.774	1.00	27.93	B	N
ATOM	3576	CA	ALA	B	971	−15.222	30.189	22.193	1.00	29.28	B	C
ATOM	3577	CB	ALA	B	971	−15.618	31.631	21.926	1.00	28.90	B	C
ATOM	3578	C	ALA	B	971	−16.220	29.252	21.519	1.00	30.92	B	C
ATOM	3579	O	ALA	B	971	−17.003	28.584	22.193	1.00	33.05	B	O
ATOM	3580	N	LYS	B	972	−16.189	29.209	20.188	1.00	30.45	B	N
ATOM	3581	CA	LYS	B	972	−17.083	28.348	19.419	1.00	30.30	B	C
ATOM	3582	CB	LYS	B	972	−16.811	28.512	17.915	1.00	32.31	B	C
ATOM	3583	CG	LYS	B	972	−17.115	29.900	17.374	1.00	33.11	B	C
ATOM	3584	CD	LYS	B	972	−18.541	30.263	17.675	1.00	35.45	B	C
ATOM	3585	CE	LYS	B	972	−18.803	31.733	17.461	1.00	38.07	B	C
ATOM	3586	NZ	LYS	B	972	−20.202	32.046	17.893	1.00	40.65	B	N
ATOM	3587	C	LYS	B	972	−16.968	26.868	19.795	1.00	29.76	B	C
ATOM	3588	O	LYS	B	972	−17.890	26.094	19.553	1.00	29.15	B	O
ATOM	3589	N	LEU	B	973	−15.837	26.473	20.375	1.00	29.72	B	N
ATOM	3590	CA	LEU	B	973	−15.630	25.078	20.766	1.00	29.44	B	C
ATOM	3591	CB	LEU	B	973	−14.195	24.643	20.436	1.00	28.00	B	C
ATOM	3592	CG	LEU	B	973	−13.825	24.196	19.010	1.00	28.81	B	C
ATOM	3593	CD1	LEU	B	973	−14.845	24.746	18.014	1.00	30.28	B	C
ATOM	3594	CD2	LEU	B	973	−12.403	24.649	18.659	1.00	24.48	B	C
ATOM	3595	C	LEU	B	973	−15.900	24.803	22.246	1.00	31.37	B	C
ATOM	3596	O	LEU	B	973	−15.989	23.647	22.649	1.00	30.12	B	O
ATOM	3597	N	LEU	B	974	−16.027	25.854	23.057	1.00	32.64	B	N
ATOM	3598	CA	LEU	B	974	−16.243	25.666	24.487	1.00	34.63	B	C
ATOM	3599	CB	LEU	B	974	−15.721	26.865	25.283	1.00	33.19	B	C
ATOM	3600	CG	LEU	B	974	−14.238	27.196	25.105	1.00	30.52	B	C
ATOM	3601	CD1	LEU	B	974	−13.887	28.402	25.940	1.00	30.49	B	C
ATOM	3602	CD2	LEU	B	974	−13.392	25.993	25.471	1.00	28.88	B	C
ATOM	3603	C	LEU	B	974	−17.681	25.399	24.870	1.00	38.43	B	C
ATOM	3604	O	LEU	B	974	−18.615	26.000	24.340	1.00	38.84	B	O
ATOM	3605	N	PRO	B	975	−17.873	24.500	25.836	1.00	42.06	B	N
ATOM	3606	CD	PRO	B	975	−16.847	23.998	26.771	1.00	40.92	B	C
ATOM	3607	CA	PRO	B	975	−19.211	24.148	26.295	1.00	42.75	B	C
ATOM	3608	CB	PRO	B	975	−18.925	23.212	27.466	1.00	43.15	B	C
ATOM	3609	CG	PRO	B	975	−17.649	23.768	28.024	1.00	41.14	B	C
ATOM	3610	C	PRO	B	975	−20.055	25.354	26.694	1.00	44.41	B	C
ATOM	3611	O	PRO	B	975	−19.644	26.179	27.501	1.00	45.61	B	O
ATOM	3612	N	LEU	B	976	−21.238	25.453	26.103	1.00	46.22	B	N
ATOM	3613	CA	LEU	B	976	−22.163	26.529	26.412	1.00	47.83	B	C
ATOM	3614	CB	LEU	B	976	−23.509	26.249	25.723	1.00	48.67	B	C
ATOM	3615	CG	LEU	B	976	−23.555	26.755	24.275	1.00	49.00	B	C
ATOM	3616	CD1	LEU	B	976	−23.755	28.270	24.297	1.00	48.21	B	C
ATOM	3617	CD2	LEU	B	976	−22.231	26.379	23.542	1.00	48.02	B	C
ATOM	3618	C	LEU	B	976	−22.340	26.661	27.929	1.00	48.28	B	C
ATOM	3619	O	LEU	B	976	−21.939	27.668	28.520	1.00	48.72	B	O
ATOM	3620	N	ASP	B	977	−22.925	25.646	28.560	1.00	48.12	B	N
ATOM	3621	CA	ASP	B	977	−23.113	25.678	30.007	1.00	48.62	B	C
ATOM	3622	CB	ASP	B	977	−24.536	25.268	30.380	1.00	50.40	B	C
ATOM	3623	CG	ASP	B	977	−24.668	24.898	31.863	1.00	53.25	B	C
ATOM	3624	OD1	ASP	B	977	−25.490	25.542	32.578	1.00	53.02	B	O

TABLE 2-continued

ATOM	3625	OD2	ASP	B	977	−23.943	23.959	32.302	1.00	53.55	B	O
ATOM	3626	C	ASP	B	977	−22.145	24.730	30.704	1.00	48.29	B	C
ATOM	3627	O	ASP	B	977	−22.227	23.513	30.525	1.00	48.69	B	O
ATOM	3628	N	LYS	B	978	−21.232	25.273	31.502	1.00	47.40	B	N
ATOM	3629	CA	LYS	B	978	−20.272	24.430	32.223	1.00	47.27	B	C
ATOM	3630	CB	LYS	B	978	−18.848	24.663	31.710	1.00	46.05	B	C
ATOM	3631	CG	LYS	B	978	−18.223	25.970	32.220	1.00	44.25	B	C
ATOM	3632	CD	LYS	B	978	−16.986	25.663	33.059	1.00	42.04	B	C
ATOM	3633	CE	LYS	B	978	−15.979	24.889	32.225	1.00	40.46	B	C
ATOM	3634	NZ	LYS	B	978	−14.751	24.538	32.986	1.00	39.42	B	N
ATOM	3635	C	LYS	B	978	−20.297	24.745	33.717	1.00	46.58	B	C
ATOM	3636	O	LYS	B	978	−20.163	25.903	34.116	1.00	46.31	B	O
ATOM	3637	N	ASP	B	979	−20.458	23.716	34.539	1.00	47.40	B	N
ATOM	3638	CA	ASP	B	979	−20.485	23.904	35.984	1.00	47.45	B	C
ATOM	3639	CB	ASP	B	979	−20.788	22.577	36.677	1.00	49.65	B	C
ATOM	3640	CG	ASP	B	979	−21.116	22.747	38.138	1.00	50.70	B	C
ATOM	3641	OD1	ASP	B	979	−21.512	21.737	38.765	1.00	51.90	B	O
ATOM	3642	OD2	ASP	B	979	−20.977	23.883	38.651	1.00	50.64	B	O
ATOM	3643	C	ASP	B	979	−19.140	24.437	36.453	1.00	46.35	B	C
ATOM	3644	O	ASP	B	979	−18.150	23.702	36.515	1.00	44.91	B	O
ATOM	3645	N	TYR	B	980	−19.115	25.724	36.781	1.00	45.52	B	N
ATOM	3646	CA	TYR	B	980	−17.897	26.383	37.230	1.00	45.44	B	C
ATOM	3647	CB	TYR	B	980	−18.069	27.899	37.131	1.00	43.35	B	C
ATOM	3648	CG	TYR	B	980	−17.833	28.436	35.739	1.00	41.95	B	C
ATOM	3649	CD1	TYR	B	980	−16.548	28.502	35.207	1.00	39.92	B	C
ATOM	3650	CE1	TYR	B	980	−16.326	28.968	33.918	1.00	37.64	B	C
ATOM	3651	CD2	TYR	B	980	−18.893	28.851	34.944	1.00	39.33	B	C
ATOM	3652	CE2	TYR	B	980	−18.683	29.317	33.654	1.00	37.16	B	C
ATOM	3653	CZ	TYR	B	980	−17.401	29.374	33.144	1.00	36.17	B	C
ATOM	3654	OH	TYR	B	980	−17.205	29.827	31.859	1.00	32.46	B	O
ATOM	3655	C	TYR	B	980	−17.431	26.006	38.635	1.00	46.34	B	C
ATOM	3656	O	TYR	B	980	−16.342	26.403	39.061	1.00	47.06	B	O
ATOM	3657	N	TYR	B	981	−18.235	25.229	39.351	1.00	46.87	B	N
ATOM	3658	CA	TYR	B	981	−17.856	24.830	40.696	1.00	48.41	B	C
ATOM	3659	CB	TYR	B	981	−19.096	24.676	41.570	1.00	50.55	B	C
ATOM	3660	CG	TYR	B	981	−19.918	25.940	41.626	1.00	54.49	B	C
ATOM	3661	CD1	TYR	B	981	−20.882	26.207	40.655	1.00	56.05	B	C
ATOM	3662	CE1	TYR	B	981	−21.594	27.398	40.656	1.00	57.69	B	C
ATOM	3663	CD2	TYR	B	981	−19.689	26.902	42.610	1.00	55.62	B	C
ATOM	3664	CE2	TYR	B	981	−20.397	28.101	42.620	1.00	57.77	B	C
ATOM	3665	CZ	TYR	B	981	−21.347	28.340	41.638	1.00	58.18	B	C
ATOM	3666	OH	TYR	B	981	−22.043	29.525	41.629	1.00	59.14	B	O
ATOM	3667	C	TYR	B	981	−17.037	23.551	40.688	1.00	47.81	B	C
ATOM	3668	O	TYR	B	981	−16.376	23.211	41.674	1.00	47.25	B	O
ATOM	3669	N	VAL	B	982	−17.076	22.850	39.563	1.00	47.13	B	N
ATOM	3670	CA	VAL	B	982	−16.317	21.621	39.411	1.00	46.15	B	C
ATOM	3671	CB	VAL	B	982	−17.082	20.599	38.547	1.00	45.79	B	C
ATOM	3672	CG1	VAL	B	982	−16.290	19.319	38.426	1.00	44.97	B	C
ATOM	3673	CG2	VAL	B	982	−18.435	20.316	39.161	1.00	45.38	B	C
ATOM	3674	C	VAL	B	982	−14.993	21.971	38.735	1.00	46.37	B	C
ATOM	3675	O	VAL	B	982	−14.864	21.867	37.515	1.00	46.84	B	O
ATOM	3676	N	VAL	B	983	−14.021	22.401	39.537	1.00	46.67	B	N
ATOM	3677	CA	VAL	B	983	−12.703	22.774	39.031	1.00	47.04	B	C
ATOM	3678	CB	VAL	B	983	−12.512	24.313	39.075	1.00	47.43	B	C
ATOM	3679	CG1	VAL	B	983	−12.785	24.836	40.482	1.00	45.36	B	C
ATOM	3680	CG2	VAL	B	983	−11.109	24.681	38.614	1.00	44.47	B	C
ATOM	3681	C	VAL	B	983	−11.594	22.095	39.837	1.00	47.73	B	C
ATOM	3682	O	VAL	B	983	−11.692	21.968	41.054	1.00	48.13	B	O
ATOM	3683	N	ARG	B	984	−10.545	21.652	39.148	1.00	48.65	B	N
ATOM	3684	CA	ARG	B	984	−9.426	20.974	39.795	1.00	49.00	B	C
ATOM	3685	CB	ARG	B	984	−8.537	20.288	38.746	1.00	51.15	B	C
ATOM	3686	CG	ARG	B	984	−8.174	18.838	39.065	1.00	54.57	B	C
ATOM	3687	CD	ARG	B	984	−7.740	18.701	40.513	1.00	59.55	B	C
ATOM	3688	NE	ARG	B	984	−7.279	17.355	40.849	1.00	62.55	B	N
ATOM	3689	CZ	ARG	B	984	−6.104	16.851	40.487	1.00	64.30	B	C
ATOM	3690	NH1	ARG	B	984	−5.780	15.614	40.843	1.00	65.05	B	N
ATOM	3691	NH2	ARG	B	984	−5.252	17.582	39.776	1.00	63.24	B	N
ATOM	3692	C	ARG	B	984	−8.594	21.966	40.598	1.00	48.48	B	C
ATOM	3693	O	ARG	B	984	−7.965	21.602	41.593	1.00	49.43	B	O
ATOM	3694	N	GLU	B	985	−8.581	23.219	40.161	1.00	46.65	B	N
ATOM	3695	CA	GLU	B	985	−7.828	24.248	40.861	1.00	43.97	B	C
ATOM	3696	CB	GLU	B	985	−6.458	24.443	40.208	1.00	45.70	B	C
ATOM	3697	CG	GLU	B	985	−5.408	25.041	41.147	1.00	51.85	B	C
ATOM	3698	CD	GLU	B	985	−4.850	24.038	42.161	1.00	53.27	B	C
ATOM	3699	OE1	GLU	B	985	−4.300	24.479	43.195	1.00	54.45	B	O
ATOM	3700	OE2	GLU	B	985	−4.944	22.814	41.921	1.00	55.23	B	O
ATOM	3701	C	GLU	B	985	−8.625	25.542	40.811	1.00	41.24	B	C
ATOM	3702	O	GLU	B	985	−8.401	26.387	39.947	1.00	40.60	B	O
ATOM	3703	N	PRO	B	986	−9.564	25.712	41.756	1.00	38.73	B	N
ATOM	3704	CD	PRO	B	986	−9.658	24.841	42.939	1.00	37.63	B	C

TABLE 2-continued

ATOM	3705	CA	PRO	B	986	−10.456	26.869	41.903	1.00	37.13	B	C
ATOM	3706	CB	PRO	B	986	−11.165	26.589	43.231	1.00	35.86	B	C
ATOM	3707	CG	PRO	B	986	−10.161	25.801	43.991	1.00	36.53	B	C
ATOM	3708	C	PRO	B	986	−9.799	28.258	41.853	1.00	36.29	B	C
ATOM	3709	O	PRO	B	986	−10.418	29.220	41.405	1.00	36.29	B	O
ATOM	3710	N	GLY	B	987	−8.557	28.372	42.310	1.00	34.80	B	N
ATOM	3711	CA	GLY	B	987	−7.900	29.665	42.266	1.00	32.48	B	C
ATOM	3712	C	GLY	B	987	−7.729	30.195	40.848	1.00	30.71	B	C
ATOM	3713	O	GLY	B	987	−7.573	31.397	40.654	1.00	28.46	B	O
ATOM	3714	N	GLN	B	988	−7.750	29.298	39.862	1.00	28.88	B	N
ATOM	3715	CA	GLN	B	988	−7.593	29.674	38.461	1.00	27.63	B	C
ATOM	3716	CB	GLN	B	988	−6.546	28.788	37.791	1.00	28.47	B	C
ATOM	3717	CG	GLN	B	988	−5.165	28.913	38.413	1.00	29.70	B	C
ATOM	3718	CD	GLN	B	988	−4.569	30.293	38.220	1.00	29.60	B	C
ATOM	3719	OE1	GLN	B	988	−4.197	30.621	37.078	1.00	25.73	B	O
ATOM	3720	NE2	GLN	B	988	−4.484	31.049	39.212	1.00	31.49	B	O
ATOM	3721	C	GLN	B	988	−8.904	29.588	37.688	1.00	28.49	B	C
ATOM	3722	O	GLN	B	988	−8.904	29.479	36.460	1.00	26.59	B	O
ATOM	3723	N	SER	B	989	−10.017	29.625	38.421	1.00	29.21	B	N
ATOM	3724	CA	SER	B	989	−11.344	29.581	37.824	1.00	29.21	B	C
ATOM	3725	CB	SER	B	989	−12.427	29.566	38.896	1.00	28.70	B	C
ATOM	3726	OG	SER	B	989	−13.694	29.771	38.300	1.00	29.29	B	O
ATOM	3727	C	SER	B	989	−11.505	30.833	36.982	1.00	29.58	B	C
ATOM	3728	O	SER	B	989	−11.334	31.945	37.474	1.00	30.64	B	O
ATOM	3729	N	PRO	B	990	−11.860	30.666	35.703	1.00	29.48	B	N
ATOM	3730	CD	PRO	B	990	−12.224	29.381	35.078	1.00	29.21	B	C
ATOM	3731	CA	PRO	B	990	−12.044	31.775	34.762	1.00	29.66	B	C
ATOM	3732	CB	PRO	B	990	−12.692	31.095	33.555	1.00	30.57	B	C
ATOM	3733	CG	PRO	B	990	−12.097	29.698	33.609	1.00	30.85	B	C
ATOM	3734	C	PRO	B	990	−12.865	32.951	35.278	1.00	27.44	B	C
ATOM	3735	O	PRO	B	990	−12.640	34.081	34.856	1.00	28.69	B	O
ATOM	3736	N	ILE	B	991	−13.807	32.689	36.180	1.00	25.37	B	N
ATOM	3737	CA	ILE	B	991	−14.656	33.751	36.717	1.00	24.21	B	C
ATOM	3738	CB	ILE	B	991	−15.636	33.216	37.789	1.00	22.18	B	C
ATOM	3739	CG2	ILE	B	991	−16.408	32.041	37.252	1.00	21.00	B	C
ATOM	3740	CG1	ILE	B	991	−14.872	32.797	39.037	1.00	22.49	B	C
ATOM	3741	CD1	ILE	B	991	−15.770	32.280	40.129	1.00	20.47	B	C
ATOM	3742	C	ILE	B	991	−13.915	34.956	37.318	1.00	22.89	B	C
ATOM	3743	O	ILE	B	991	−14.380	36.084	37.184	1.00	22.11	B	O
ATOM	3744	N	PHE	B	992	−12.771	34.738	37.961	1.00	20.98	B	N
ATOM	3745	CA	PHE	B	992	−12.052	35.867	38.555	1.00	21.73	B	C
ATOM	3746	CB	PHE	B	992	−10.972	35.365	39.528	1.00	19.62	B	C
ATOM	3747	CG	PHE	B	992	−11.520	34.512	40.634	1.00	18.15	B	C
ATOM	3748	CD1	PHE	B	992	−12.614	34.947	41.378	1.00	17.59	B	C
ATOM	3749	CD2	PHE	B	992	−10.968	33.272	40.912	1.00	16.48	B	C
ATOM	3750	CE1	PHE	B	992	−13.154	34.162	42.379	1.00	17.22	B	C
ATOM	3751	CE2	PHE	B	992	−11.495	32.476	41.909	1.00	18.83	B	C
ATOM	3752	CZ	PHE	B	992	−12.596	32.921	42.650	1.00	18.84	B	C
ATOM	3753	C	PHE	B	992	−11.439	36.841	37.544	1.00	21.99	B	C
ATOM	3754	O	PHE	B	992	−10.912	37.884	37.933	1.00	21.24	B	O
ATOM	3755	N	TRP	B	993	−11.520	36.494	36.257	1.00	21.93	B	N
ATOM	3756	CA	TRP	B	993	−11.004	37.325	35.159	1.00	23.05	B	C
ATOM	3757	CB	TRP	B	993	−10.049	36.515	34.275	1.00	19.09	B	C
ATOM	3758	CG	TRP	B	993	−8.689	36.325	34.848	1.00	20.94	B	C
ATOM	3759	CD2	TRP	B	993	−8.296	35.374	35.852	1.00	20.70	B	C
ATOM	3760	CE2	TRP	B	993	−6.932	35.608	36.129	1.00	20.32	B	C
ATOM	3761	CE3	TRP	B	993	−8.965	34.348	36.541	1.00	20.74	B	C
ATOM	3762	CD1	TRP	B	993	−7.579	37.065	34.568	1.00	21.22	B	C
ATOM	3763	NE1	TRP	B	993	−6.523	36.644	35.336	1.00	22.28	B	N
ATOM	3764	CZ2	TRP	B	993	−6.222	34.857	37.073	1.00	18.70	B	C
ATOM	3765	CZ3	TRP	B	993	−8.257	33.602	37.479	1.00	16.48	B	C
ATOM	3766	CH2	TRP	B	993	−6.897	33.864	37.734	1.00	17.27	B	C
ATOM	3767	C	TRP	B	993	−12.153	37.841	34.288	1.00	24.85	B	C
ATOM	3768	O	TRP	B	993	−11.966	38.714	33.436	1.00	26.79	B	O
ATOM	3769	N	TYR	B	994	−13.347	37.307	34.506	1.00	25.07	B	N
ATOM	3770	CA	TYR	B	994	−14.492	37.685	33.689	1.00	25.56	B	C
ATOM	3771	CB	TYR	B	994	−15.661	36.721	33.929	1.00	26.05	B	C
ATOM	3772	CG	TYR	B	994	−15.487	35.343	33.314	1.00	26.17	B	C
ATOM	3773	CD1	TYR	B	994	−14.323	35.005	32.624	1.00	25.80	B	C
ATOM	3774	CE1	TYR	B	994	−14.189	33.761	32.008	1.00	26.46	B	C
ATOM	3775	CD2	TYR	B	994	−16.510	34.397	33.376	1.00	26.01	B	C
ATOM	3776	CE2	TYR	B	994	−16.384	33.153	32.763	1.00	25.93	B	C
ATOM	3777	CZ	TYR	B	994	−15.223	32.840	32.079	1.00	26.41	B	C
ATOM	3778	OH	TYR	B	994	−15.090	31.616	31.458	1.00	27.87	B	O
ATOM	3779	C	TYR	B	994	−14.981	39.095	33.902	1.00	25.85	B	C
ATOM	3780	O	TYR	B	994	−15.005	39.587	35.020	1.00	27.26	B	O
ATOM	3781	N	ALA	B	995	−15.369	39.752	32.816	1.00	26.65	B	N
ATOM	3782	CA	ALA	B	995	−15.911	41.094	32.925	1.00	25.40	B	C
ATOM	3783	CB	ALA	B	995	−15.883	41.789	31.578	1.00	23.16	B	C
ATOM	3784	C	ALA	B	995	−17.352	40.907	33.389	1.00	25.46	B	C

TABLE 2-continued

ATOM	3785	O	ALA	B	995	−17.916	39.813	33.284	1.00	23.51	B	O
ATOM	3786	N	PRO	B	996	−17.963	41.970	33.917	1.00	25.58	B	N
ATOM	3787	CD	PRO	B	996	−17.400	43.304	34.173	1.00	25.53	B	C
ATOM	3788	CA	PRO	B	996	−19.344	41.893	34.389	1.00	27.00	B	C
ATOM	3789	CB	PRO	B	996	−19.683	43.349	34.682	1.00	24.54	B	C
ATOM	3790	CG	PRO	B	996	−18.395	43.888	35.131	1.00	24.67	B	C
ATOM	3791	C	PRO	B	996	−20.303	41.263	33.374	1.00	28.59	B	C
ATOM	3792	O	PRO	B	996	−20.943	40.252	33.674	1.00	28.72	B	O
ATOM	3793	N	GLU	B	997	−20.391	41.850	32.179	1.00	29.28	B	N
ATOM	3794	CA	GLU	B	997	−21.301	41.342	31.153	1.00	30.88	B	C
ATOM	3795	CB	GLU	B	997	−21.101	42.057	29.798	1.00	31.68	B	C
ATOM	3796	CG	GLU	B	997	−19.734	41.900	29.169	1.00	30.63	B	C
ATOM	3797	CD	GLU	B	997	−18.779	42.982	29.608	1.00	32.64	B	C
ATOM	3798	OE1	GLU	B	997	−18.945	43.483	30.745	1.00	31.73	B	O
ATOM	3799	OE2	GLU	B	997	−17.864	43.322	28.822	1.00	31.67	B	O
ATOM	3800	C	GLU	B	997	−21.134	39.847	30.963	1.00	31.40	B	C
ATOM	3801	O	GLU	B	997	−22.082	39.151	30.611	1.00	31.19	B	O
ATOM	3802	N	SER	B	998	−19.926	39.348	31.202	1.00	31.66	B	N
ATOM	3803	CA	SER	B	998	−19.676	37.923	31.053	1.00	30.81	B	C
ATOM	3804	CB	SER	B	998	−18.178	37.633	31.053	1.00	29.42	B	C
ATOM	3805	OG	SER	B	998	−17.611	37.933	29.793	1.00	30.14	B	O
ATOM	3806	C	SER	B	998	−20.343	37.131	32.159	1.00	30.19	B	C
ATOM	3807	O	SER	B	998	−20.926	36.081	31.911	1.00	32.24	B	O
ATOM	3808	N	LEU	B	999	−20.261	37.631	33.381	1.00	31.65	B	N
ATOM	3809	CA	LEU	B	999	−20.854	36.931	34.508	1.00	33.55	B	C
ATOM	3810	CB	LEU	B	999	−20.399	37.560	35.828	1.00	30.58	B	C
ATOM	3811	CG	LEU	B	999	−18.949	37.373	36.287	1.00	30.41	B	C
ATOM	3812	CD1	LEU	B	999	−18.792	37.992	37.667	1.00	29.34	B	C
ATOM	3813	CD2	LEU	B	999	−18.595	35.904	36.351	1.00	28.97	B	C
ATOM	3814	C	LEU	B	999	−22.378	36.909	34.458	1.00	35.12	B	C
ATOM	3815	O	LEU	B	999	−22.999	35.902	34.788	1.00	35.62	B	O
ATOM	3816	N	SER	B	1000	−22.982	38.014	34.039	1.00	36.04	B	N
ATOM	3817	CA	SER	B	1000	−24.433	38.094	33.986	1.00	37.54	B	C
ATOM	3818	CB	SER	B	1000	−24.889	39.515	34.319	1.00	38.20	B	C
ATOM	3819	OG	SER	B	1000	−24.368	40.453	33.391	1.00	39.11	B	O
ATOM	3820	C	SER	B	1000	−25.076	37.677	32.671	1.00	38.49	B	C
ATOM	3821	O	SER	B	1000	−26.296	37.563	32.603	1.00	38.27	B	O
ATOM	3822	N	ASP	B	1001	−24.279	37.445	31.633	1.00	38.91	B	N
ATOM	3823	CA	ASP	B	1001	−24.847	37.075	30.339	1.00	41.24	B	C
ATOM	3824	CB	ASP	B	1001	−25.201	38.350	29.573	1.00	42.19	B	C
ATOM	3825	CG	ASP	B	1001	−26.330	39.118	30.220	1.00	44.29	B	C
ATOM	3826	OD1	ASP	B	1001	−27.446	38.561	30.286	1.00	43.63	B	O
ATOM	3827	OD2	ASP	B	1001	−26.103	40.271	30.660	1.00	45.40	B	O
ATOM	3828	C	ASP	B	1001	−24.001	36.167	29.434	1.00	41.18	B	C
ATOM	3829	O	ASP	B	1001	−24.409	35.859	28.313	1.00	39.87	B	O
ATOM	3830	N	ASN	B	1002	−22.839	35.735	29.914	1.00	40.49	B	N
ATOM	3831	CA	ASN	B	1002	−21.952	34.892	29.118	1.00	41.92	B	C
ATOM	3832	CB	ASN	B	1002	−22.680	33.636	28.625	1.00	43.88	B	C
ATOM	3833	CG	ASN	B	1002	−23.039	32.696	29.748	1.00	47.49	B	C
ATOM	3834	OD1	ASN	B	1002	−22.165	32.216	30.465	1.00	50.58	B	O
ATOM	3835	ND2	ASN	B	1002	−24.331	32.425	29.911	1.00	48.38	B	N
ATOM	3836	C	ASN	B	1002	−21.415	35.668	27.916	1.00	42.17	B	C
ATOM	3837	O	ASN	B	1002	−20.720	35.109	27.072	1.00	42.74	B	O
ATOM	3838	N	ILE	B	1003	−21.737	36.958	27.850	1.00	40.60	B	N
ATOM	3839	CA	ILE	B	1003	−21.293	37.822	26.760	1.00	37.90	B	C
ATOM	3840	CB	ILE	B	1003	−21.949	39.218	26.855	1.00	38.42	B	C
ATOM	3841	CG2	ILE	B	1003	−21.375	40.150	25.821	1.00	35.41	B	C
ATOM	3842	CG1	ILE	B	1003	−23.456	39.099	26.667	1.00	38.11	B	C
ATOM	3843	CD1	ILE	B	1003	−24.163	40.422	26.794	1.00	36.73	B	C
ATOM	3844	C	ILE	B	1003	−19.781	38.007	26.777	1.00	37.25	B	C
ATOM	3845	O	ILE	B	1003	−19.209	38.409	27.791	1.00	38.16	B	O
ATOM	3846	N	PHE	B	1004	−19.143	37.710	25.649	1.00	34.80	B	N
ATOM	3847	CA	PHE	B	1004	−17.701	37.846	25.505	1.00	33.02	B	C
ATOM	3848	CB	PHE	B	1004	−17.053	36.468	25.379	1.00	31.30	B	C
ATOM	3849	CG	PHE	B	1004	−17.010	35.695	26.672	1.00	33.33	B	C
ATOM	3850	CD1	PHE	B	1004	−16.122	36.053	27.681	1.00	31.07	B	C
ATOM	3851	CD2	PHE	B	1004	−17.871	34.619	26.889	1.00	33.88	B	C
ATOM	3852	CE1	PHE	B	1004	−16.088	35.360	28.882	1.00	31.19	B	C
ATOM	3853	CE2	PHE	B	1004	−17.848	33.913	28.094	1.00	33.73	B	C
ATOM	3854	CZ	PHE	B	1004	−16.953	34.284	29.094	1.00	31.84	B	C
ATOM	3855	C	PHE	B	1004	−17.416	38.672	24.261	1.00	33.61	B	C
ATOM	3856	O	PHE	B	1004	−18.005	38.426	23.214	1.00	36.40	B	O
ATOM	3857	N	SER	B	1005	−16.521	39.651	24.373	1.00	32.85	B	N
ATOM	3858	CA	SER	B	1005	−16.181	40.507	23.243	1.00	31.81	B	C
ATOM	3859	CB	SER	B	1005	−17.128	41.697	23.178	1.00	32.82	B	C
ATOM	3860	OG	SER	B	1005	−16.862	42.582	24.254	1.00	35.29	B	O
ATOM	3861	C	SER	B	1005	−14.764	41.038	23.368	1.00	31.55	B	C
ATOM	3862	O	SER	B	1005	−14.071	40.758	24.346	1.00	30.74	B	O
ATOM	3863	N	ARG	B	1006	−14.342	41.811	22.371	1.00	30.35	B	N
ATOM	3864	CA	ARG	B	1006	−13.010	42.399	22.375	1.00	31.73	B	C

TABLE 2-continued

ATOM	3865	CB	ARG	B	1006	−12.791	43.233	21.103	1.00	32.08	B	C
ATOM	3866	CG	ARG	B	1006	−12.340	42.401	19.909	1.00	35.73	B	C
ATOM	3867	CD	ARG	B	1006	−12.529	43.117	18.571	1.00	38.23	B	C
ATOM	3868	NE	ARG	B	1006	−11.797	44.376	18.500	1.00	42.85	B	N
ATOM	3869	CZ	ARG	B	1006	−11.646	45.100	17.393	1.00	43.99	B	C
ATOM	3870	NH1	ARG	B	1006	−10.968	46.238	17.433	1.00	42.77	B	N
ATOM	3871	NH2	ARG	B	1006	−12.159	44.681	16.244	1.00	45.31	B	N
ATOM	3872	C	ARG	B	1006	−12.836	43.273	23.612	1.00	31.29	B	C
ATOM	3873	O	ARG	B	1006	−11.750	43.352	24.191	1.00	30.22	B	O
ATOM	3874	N	GLN	B	1007	−13.924	43.910	24.029	1.00	30.47	B	N
ATOM	3875	CA	GLN	B	1007	−13.881	44.788	25.184	1.00	28.48	B	C
ATOM	3876	CB	GLN	B	1007	−15.064	45.757	25.139	1.00	29.31	B	C
ATOM	3877	CG	GLN	B	1007	−14.935	46.827	24.039	1.00	30.12	B	C
ATOM	3878	CD	GLN	B	1007	−13.647	47.677	24.155	1.00	31.23	B	C
ATOM	3879	OE1	GLN	B	1007	−12.602	47.362	23.559	1.00	24.82	B	O
ATOM	3880	NE2	GLN	B	1007	−13.729	48.756	24.936	1.00	29.95	B	N
ATOM	3881	C	GLN	B	1007	−13.838	44.033	26.509	1.00	26.99	B	C
ATOM	3882	O	GLN	B	1007	−13.243	44.505	27.478	1.00	25.04	B	O
ATOM	3883	N	SER	B	1008	−14.468	42.865	26.559	1.00	25.68	B	N
ATOM	3884	CA	SER	B	1008	−14.434	42.057	27.772	1.00	26.10	B	C
ATOM	3885	CB	SER	B	1008	−15.421	40.891	27.665	1.00	27.87	B	C
ATOM	3886	OG	SER	B	1008	−15.080	40.026	26.598	1.00	31.41	B	O
ATOM	3887	C	SER	B	1008	−12.995	41.538	27.944	1.00	26.67	B	C
ATOM	3888	O	SER	B	1008	−12.501	41.384	29.065	1.00	26.79	B	O
ATOM	3889	N	ASP	B	1009	−12.324	41.265	26.825	1.00	25.33	B	N
ATOM	3890	CA	ASP	B	1009	−10.943	40.806	26.872	1.00	25.36	B	C
ATOM	3891	CB	ASP	B	1009	−10.409	40.469	25.468	1.00	26.35	B	C
ATOM	3892	CG	ASP	B	1009	−10.917	39.121	24.942	1.00	29.84	B	C
ATOM	3893	OD1	ASP	B	1009	−10.675	38.823	23.742	1.00	30.40	B	O
ATOM	3894	OD2	ASP	B	1009	−11.543	38.365	25.723	1.00	28.13	B	O
ATOM	3895	C	ASP	B	1009	−10.105	41.926	27.472	1.00	24.93	B	C
ATOM	3896	O	ASP	B	1009	−9.102	41.680	28.143	1.00	24.99	B	O
ATOM	3897	N	VAL	B	1010	−10.524	43.162	27.228	1.00	22.69	B	N
ATOM	3898	CA	VAL	B	1010	−9.797	44.307	27.751	1.00	23.10	B	C
ATOM	3899	CB	VAL	B	1010	−10.400	45.641	27.246	1.00	21.13	B	C
ATOM	3900	CG1	VAL	B	1010	−9.916	46.783	28.110	1.00	21.03	B	C
ATOM	3901	CG2	VAL	B	1010	−9.992	45.886	25.803	1.00	18.23	B	C
ATOM	3902	C	VAL	B	1010	−9.823	44.278	29.277	1.00	23.05	B	C
ATOM	3903	O	VAL	B	1010	−8.823	44.568	29.927	1.00	22.50	B	O
ATOM	3904	N	TRP	B	1011	−10.977	43.924	29.833	1.00	23.37	B	N
ATOM	3905	CA	TRP	B	1011	−11.156	43.834	31.274	1.00	22.16	B	C
ATOM	3906	CB	TRP	B	1011	−12.605	43.436	31.582	1.00	21.39	B	C
ATOM	3907	CG	TRP	B	1011	−12.856	43.017	33.021	1.00	22.17	B	C
ATOM	3908	CD2	TRP	B	1011	−13.633	43.722	33.994	1.00	21.79	B	C
ATOM	3909	CE2	TRP	B	1011	−13.611	42.956	35.187	1.00	22.59	B	C
ATOM	3910	CE3	TRP	B	1011	−14.346	44.924	33.977	1.00	20.63	B	C
ATOM	3911	CD1	TRP	B	1011	−12.400	41.885	33.647	1.00	21.99	B	C
ATOM	3912	NE1	TRP	B	1011	−12.851	41.840	34.946	1.00	20.90	B	N
ATOM	3913	CZ2	TRP	B	1011	−14.276	43.353	36.350	1.00	22.92	B	C
ATOM	3914	CZ3	TRP	B	1011	−15.006	45.318	35.130	1.00	22.87	B	C
ATOM	3915	CH2	TRP	B	1011	−14.966	44.532	36.302	1.00	24.34	B	C
ATOM	3916	C	TRP	B	1011	−10.199	42.783	31.832	1.00	22.62	B	C
ATOM	3917	O	TRP	B	1011	−9.496	43.006	32.818	1.00	22.51	B	O
ATOM	3918	N	SER	B	1012	−10.184	41.628	31.185	1.00	23.22	B	N
ATOM	3919	CA	SER	B	1012	−9.329	40.540	31.614	1.00	21.86	B	C
ATOM	3920	CB	SER	B	1012	−9.583	39.315	30.745	1.00	23.31	B	C
ATOM	3921	OG	SER	B	1012	−10.969	39.024	30.712	1.00	26.28	B	O
ATOM	3922	C	SER	B	1012	−7.869	40.952	31.547	1.00	20.42	B	C
ATOM	3923	O	SER	B	1012	−7.054	40.446	32.312	1.00	19.32	B	O
ATOM	3924	N	PHE	B	1013	−7.544	41.864	30.630	1.00	19.51	B	N
ATOM	3925	CA	PHE	B	1013	−6.178	42.369	30.480	1.00	20.32	B	C
ATOM	3926	CB	PHE	B	1013	−6.060	43.253	29.241	1.00	22.41	B	C
ATOM	3927	CG	PHE	B	1013	−4.738	43.954	29.127	1.00	24.71	B	C
ATOM	3928	CD1	PHE	B	1013	−3.566	43.233	28.933	1.00	25.77	B	C
ATOM	3929	CD2	PHE	B	1013	−4.660	45.335	29.215	1.00	24.66	B	C
ATOM	3930	CE1	PHE	B	1013	−2.340	43.881	28.825	1.00	25.47	B	C
ATOM	3931	CE2	PHE	B	1013	−3.441	45.992	29.109	1.00	24.49	B	C
ATOM	3932	CZ	PHE	B	1013	−2.278	45.263	28.912	1.00	24.92	B	C
ATOM	3933	C	PHE	B	1013	−5.823	43.189	31.722	1.00	20.57	B	C
ATOM	3934	O	PHE	B	1013	−4.671	43.203	32.178	1.00	18.68	B	O
ATOM	3935	N	GLY	B	1014	−6.829	43.868	32.261	1.00	18.88	B	N
ATOM	3936	CA	GLY	B	1014	−6.621	44.653	33.460	1.00	23.16	B	C
ATOM	3937	C	GLY	B	1014	−6.124	43.788	34.616	1.00	25.05	B	C
ATOM	3938	O	GLY	B	1014	−5.211	44.166	35.357	1.00	24.37	B	O
ATOM	3939	N	VAL	B	1015	−6.729	42.614	34.762	1.00	26.14	B	N
ATOM	3940	CA	VAL	B	1015	−6.365	41.681	35.819	1.00	25.90	B	C
ATOM	3941	CB	VAL	B	1015	−7.414	40.524	35.941	1.00	25.19	B	C
ATOM	3942	CG1	VAL	B	1015	−7.097	39.649	37.130	1.00	26.98	B	C
ATOM	3943	CG2	VAL	B	1015	−8.811	41.089	36.094	1.00	24.45	B	C
ATOM	3944	C	VAL	B	1015	−4.990	41.096	35.514	1.00	26.88	B	C

TABLE 2-continued

ATOM	3945	O	VAL	B	1015	−4.188	40.881	36.419	1.00	29.42	B	O
ATOM	3946	N	VAL	B	1016	−4.707	40.835	34.242	1.00	26.06	B	N
ATOM	3947	CA	VAL	B	1016	−3.401	40.296	33.874	1.00	25.47	B	C
ATOM	3948	CB	VAL	B	1016	−3.295	40.064	32.363	1.00	26.29	B	C
ATOM	3949	CG1	VAL	B	1016	−1.829	40.017	31.953	1.00	24.37	B	C
ATOM	3950	CG2	VAL	B	1016	−4.007	38.774	31.988	1.00	25.27	B	C
ATOM	3951	C	VAL	B	1016	−2.301	41.270	34.290	1.00	24.52	B	C
ATOM	3952	O	VAL	B	1016	−1.230	40.859	34.711	1.00	24.76	B	O
ATOM	3953	N	LEU	B	1017	−2.565	42.565	34.148	1.00	24.65	B	N
ATOM	3954	CA	LEU	B	1017	−1.594	43.582	34.543	1.00	24.58	B	C
ATOM	3955	CB	LEU	B	1017	−2.113	44.983	34.216	1.00	23.12	B	C
ATOM	3956	CG	LEU	B	1017	−2.027	45.460	32.761	1.00	24.37	B	C
ATOM	3957	CD1	LEU	B	1017	−2.982	46.629	32.545	1.00	23.70	B	C
ATOM	3958	CD2	LEU	B	1017	−0.601	45.846	32.420	1.00	21.72	B	C
ATOM	3959	C	LEU	B	1017	−1.373	43.457	36.042	1.00	25.27	B	C
ATOM	3960	O	LEU	B	1017	−0.257	43.645	36.540	1.00	24.20	B	O
ATOM	3961	N	TYR	B	1018	−2.452	43.132	36.752	1.00	25.30	B	N
ATOM	3962	CA	TYR	B	1018	−2.402	42.960	38.195	1.00	26.88	B	C
ATOM	3963	CB	TYR	B	1018	−3.794	42.657	38.729	1.00	26.68	B	C
ATOM	3964	CG	TYR	B	1018	−3.862	42.524	40.231	1.00	30.83	B	C
ATOM	3965	CD1	TYR	B	1018	−3.656	43.624	41.057	1.00	32.09	B	C
ATOM	3966	CE1	TYR	B	1018	−3.736	43.509	42.430	1.00	30.76	B	C
ATOM	3967	CD2	TYR	B	1018	−4.147	41.301	40.826	1.00	31.00	B	C
ATOM	3968	CE2	TYR	B	1018	−4.228	41.178	42.198	1.00	31.86	B	C
ATOM	3969	CZ	TYR	B	1018	−4.022	42.284	42.990	1.00	31.82	B	C
ATOM	3970	OH	TYR	B	1018	−4.101	42.159	44.350	1.00	33.07	B	O
ATOM	3971	C	TYR	B	1018	−1.449	41.816	38.549	1.00	28.71	B	C
ATOM	3972	O	TYR	B	1018	−0.540	41.979	39.372	1.00	29.73	B	O
ATOM	3973	N	GLU	B	1019	−1.652	40.669	37.902	1.00	29.08	B	N
ATOM	3974	CA	GLU	B	1019	−0.838	39.475	38.138	1.00	28.73	B	C
ATOM	3975	CB	GLU	B	1019	−1.273	38.322	37.212	1.00	28.24	B	C
ATOM	3976	CG	GLU	B	1019	−2.737	37.877	37.359	1.00	28.46	B	C
ATOM	3977	CD	GLU	B	1019	−3.029	36.554	36.653	1.00	29.77	B	C
ATOM	3978	OE1	GLU	B	1019	−2.463	35.518	37.057	1.00	33.63	B	O
ATOM	3979	OE2	GLU	B	1019	−3.824	36.538	35.691	1.00	30.03	B	O
ATOM	3980	C	GLU	B	1019	0.654	39.737	37.950	1.00	28.13	B	C
ATOM	3981	O	GLU	B	1019	1.475	39.295	38.759	1.00	27.79	B	O
ATOM	3982	N	LEU	B	1020	1.002	40.452	36.885	1.00	27.07	B	N
ATOM	3983	CA	LEU	B	1020	2.400	40.762	36.598	1.00	28.46	B	C
ATOM	3984	CB	LEU	B	1020	2.518	41.508	35.256	1.00	28.04	B	C
ATOM	3985	CG	LEU	B	1020	2.371	40.718	33.948	1.00	31.18	B	C
ATOM	3986	CD1	LEU	B	1020	3.729	40.598	33.271	1.00	30.88	B	C
ATOM	3987	CD2	LEU	B	1020	1.763	39.333	34.221	1.00	30.43	B	C
ATOM	3988	C	LEU	B	1020	3.054	41.592	37.709	1.00	27.19	B	C
ATOM	3989	O	LEU	B	1020	4.108	41.229	38.225	1.00	27.55	B	O
ATOM	3990	N	PHE	B	1021	2.428	42.704	38.070	1.00	27.54	B	N
ATOM	3991	CA	PHE	B	1021	2.962	43.573	39.108	1.00	30.47	B	C
ATOM	3992	CB	PHE	B	1021	2.370	44.977	38.954	1.00	29.66	B	C
ATOM	3993	CG	PHE	B	1021	2.887	45.705	37.750	1.00	32.67	B	C
ATOM	3994	CD1	PHE	B	1021	4.129	46.331	37.781	1.00	32.20	B	C
ATOM	3995	CD2	PHE	B	1021	2.190	45.673	36.556	1.00	32.11	B	C
ATOM	3996	CE1	PHE	B	1021	4.667	46.902	36.648	1.00	32.96	B	C
ATOM	3997	CE2	PHE	B	1021	2.726	46.243	35.416	1.00	34.86	B	C
ATOM	3998	CZ	PHE	B	1021	3.970	46.858	35.464	1.00	34.05	B	C
ATOM	3999	C	PHE	B	1021	2.687	43.005	40.498	1.00	31.35	B	C
ATOM	4000	O	PHE	B	1021	2.954	43.640	41.513	1.00	33.73	B	O
ATOM	4001	N	THR	B	1022	2.157	41.793	40.531	1.00	29.56	B	N
ATOM	4002	CA	THR	B	1022	1.855	41.122	41.782	1.00	27.88	B	C
ATOM	4003	CB	THR	B	1022	0.337	40.771	41.815	1.00	27.78	B	C
ATOM	4004	OG1	THR	B	1022	−0.276	41.380	42.959	1.00	29.16	B	O
ATOM	4005	CG2	THR	B	1022	0.105	39.265	41.830	1.00	27.02	B	C
ATOM	4006	C	THR	B	1022	2.725	39.857	41.774	1.00	27.55	B	C
ATOM	4007	O	THR	B	1022	2.716	39.060	42.711	1.00	25.85	B	O
ATOM	4008	N	TYR	B	1023	3.482	39.708	40.686	1.00	28.38	B	N
ATOM	4009	CA	TYR	B	1023	4.349	38.554	40.446	1.00	27.73	B	C
ATOM	4010	CB	TYR	B	1023	5.563	38.595	41.375	1.00	28.82	B	C
ATOM	4011	CG	TYR	B	1023	6.554	39.677	41.004	1.00	29.97	B	C
ATOM	4012	CD1	TYR	B	1023	6.475	40.948	41.562	1.00	30.60	B	C
ATOM	4013	CE1	TYR	B	1023	7.373	41.941	41.213	1.00	28.91	B	C
ATOM	4014	CD2	TYR	B	1023	7.558	39.432	40.083	1.00	29.49	B	C
ATOM	4015	CE2	TYR	B	1023	8.455	40.419	39.732	1.00	29.77	B	C
ATOM	4016	CZ	TYR	B	1023	8.356	41.667	40.301	1.00	29.39	B	C
ATOM	4017	OH	TYR	B	1023	9.258	42.637	39.961	1.00	29.99	B	O
ATOM	4018	C	TYR	B	1023	3.600	37.222	40.610	1.00	26.68	B	C
ATOM	4019	O	TYR	B	1023	4.210	36.154	40.690	1.00	23.68	B	O
ATOM	4020	N	CYS	B	1024	2.275	37.305	40.633	1.00	25.16	B	N
ATOM	4021	CA	CYS	B	1024	1.411	36.141	40.801	1.00	30.36	B	C
ATOM	4022	CB	CYS	B	1024	1.695	35.062	39.745	1.00	29.66	B	C
ATOM	4023	SG	CYS	B	1024	0.991	35.464	38.132	1.00	31.45	B	S
ATOM	4024	C	CYS	B	1024	1.539	35.542	42.180	1.00	31.11	B	C

TABLE 2-continued

ATOM	4025	O	CYS	B	1024	1.458	34.326	42.353	1.00	33.32	B	O
ATOM	4026	N	ASP	B	1025	1.736	36.394	43.172	1.00	30.88	B	N
ATOM	4027	CA	ASP	B	1025	1.843	35.888	44.523	1.00	32.73	B	C
ATOM	4028	CB	ASP	B	1025	2.062	37.031	45.501	1.00	35.93	B	C
ATOM	4029	CG	ASP	B	1025	2.440	36.541	46.869	1.00	39.06	B	C
ATOM	4030	OD1	ASP	B	1025	3.542	35.963	46.993	1.00	41.51	B	O
ATOM	4031	OD2	ASP	B	1025	1.637	36.723	47.809	1.00	41.43	B	O
ATOM	4032	C	ASP	B	1025	0.539	35.165	44.859	1.00	31.75	B	C
ATOM	4033	O	ASP	B	1025	−0.536	35.619	44.482	1.00	28.94	B	O
ATOM	4034	N	LYS	B	1026	0.637	34.046	45.567	1.00	33.64	B	N
ATOM	4035	CA	LYS	B	1026	−0.545	33.267	45.934	1.00	34.91	B	C
ATOM	4036	CB	LYS	B	1026	−0.140	31.856	46.378	1.00	37.07	B	C
ATOM	4037	CG	LYS	B	1026	0.308	30.944	45.244	1.00	39.64	B	C
ATOM	4038	CD	LYS	B	1026	−0.822	30.721	44.235	1.00	43.37	B	C
ATOM	4039	CE	LYS	B	1026	−0.378	29.791	43.097	1.00	45.58	B	C
ATOM	4040	NZ	LYS	B	1026	−1.366	29.696	41.972	1.00	46.97	B	N
ATOM	4041	C	LYS	B	1026	−1.358	33.928	47.035	1.00	34.73	B	C
ATOM	4042	O	LYS	B	1026	−2.544	33.653	47.184	1.00	34.89	B	O
ATOM	4043	N	SER	B	1027	−0.712	34.803	47.798	1.00	35.10	B	N
ATOM	4044	CA	SER	B	1027	−1.366	35.507	48.891	1.00	34.69	B	C
ATOM	4045	CB	SER	B	1027	−0.314	36.141	49.788	1.00	35.42	B	C
ATOM	4046	OG	SER	B	1027	0.677	35.191	50.131	1.00	39.15	B	O
ATOM	4047	C	SER	B	1027	−2.329	36.586	48.410	1.00	34.71	B	C
ATOM	4048	O	SER	B	1027	−3.418	36.741	48.960	1.00	35.34	B	O
ATOM	4049	N	CYS	B	1028	−1.935	37.335	47.386	1.00	34.72	B	N
ATOM	4050	CA	CYS	B	1028	−2.795	38.405	46.879	1.00	34.48	B	C
ATOM	4051	CB	CYS	B	1028	−2.073	39.741	47.008	1.00	34.38	B	C
ATOM	4052	SG	CYS	B	1028	−0.504	39.739	46.191	1.00	37.79	B	S
ATOM	4053	C	CYS	B	1028	−3.262	38.220	45.434	1.00	31.11	B	C
ATOM	4054	O	CYS	B	1028	−3.480	39.187	44.713	1.00	31.03	B	O
ATOM	4055	N	SER	B	1029	−3.417	36.974	45.020	1.00	30.32	B	N
ATOM	4056	CA	SER	B	1029	−3.867	36.665	43.670	1.00	29.14	B	C
ATOM	4057	CB	SER	B	1029	−3.800	35.163	43.449	1.00	29.51	B	C
ATOM	4058	OG	SER	B	1029	−4.812	34.543	44.225	1.00	32.23	B	O
ATOM	4059	C	SER	B	1029	−5.317	37.115	43.517	1.00	26.52	B	C
ATOM	4060	O	SER	B	1029	−5.968	37.498	44.489	1.00	27.24	B	O
ATOM	4061	N	PRO	B	1030	−5.839	37.062	42.287	1.00	24.08	B	N
ATOM	4062	CD	PRO	B	1030	−5.086	36.857	41.039	1.00	22.45	B	C
ATOM	4063	CA	PRO	B	1030	−7.210	37.457	41.987	1.00	23.13	B	C
ATOM	4064	CB	PRO	B	1030	−7.299	37.196	40.496	1.00	22.81	B	C
ATOM	4065	CG	PRO	B	1030	−5.934	37.581	40.043	1.00	20.71	B	C
ATOM	4066	C	PRO	B	1030	−8.262	36.702	42.796	1.00	24.05	B	C
ATOM	4067	O	PRO	B	1030	−9.180	37.309	43.374	1.00	23.62	B	O
ATOM	4068	N	SER	B	1031	−8.136	35.380	42.834	1.00	24.60	B	N
ATOM	4069	CA	SER	B	1031	−9.066	34.567	43.600	1.00	25.29	B	C
ATOM	4070	CB	SER	B	1031	−8.741	33.081	43.411	1.00	24.41	B	C
ATOM	4071	OG	SER	B	1031	−7.367	32.829	43.619	1.00	29.84	B	O
ATOM	4072	C	SER	B	1031	−9.035	34.936	45.098	1.00	26.53	B	C
ATOM	4073	O	SER	B	1031	−10.082	35.168	45.707	1.00	26.40	B	O
ATOM	4074	N	ALA	B	1032	−7.836	35.000	45.680	1.00	27.33	B	N
ATOM	4075	CA	ALA	B	1032	−7.675	35.332	47.094	1.00	27.47	B	C
ATOM	4076	CB	ALA	B	1032	−6.189	35.394	47.447	1.00	28.40	B	C
ATOM	4077	C	ALA	B	1032	−8.364	36.646	47.479	1.00	28.39	B	C
ATOM	4078	O	ALA	B	1032	−9.314	36.645	48.266	1.00	27.17	B	O
ATOM	4079	N	GLU	B	1033	−7.887	37.760	46.925	1.00	28.39	B	N
ATOM	4080	CA	GLU	B	1033	−8.474	39.073	47.208	1.00	28.46	B	C
ATOM	4081	CB	GLU	B	1033	−7.907	40.142	46.270	1.00	30.40	B	C
ATOM	4082	CG	GLU	B	1033	−6.432	40.445	46.464	1.00	34.55	B	C
ATOM	4083	CD	GLU	B	1033	−6.063	40.634	47.920	1.00	36.21	B	C
ATOM	4084	OE1	GLU	B	1033	−6.955	40.978	48.723	1.00	35.21	B	O
ATOM	4085	OE2	GLU	B	1033	−4.874	40.448	48.257	1.00	37.70	B	O
ATOM	4086	C	GLU	B	1033	−9.984	39.074	47.068	1.00	27.91	B	C
ATOM	4087	O	GLU	B	1033	−10.691	39.580	47.931	1.00	28.02	B	O
ATOM	4088	N	PHE	B	1034	−10.480	38.523	45.965	1.00	28.93	B	N
ATOM	4089	CA	PHE	B	1034	−11.917	38.466	45.728	1.00	27.01	B	C
ATOM	4090	CB	PHE	B	1034	−12.195	37.895	44.335	1.00	25.79	B	C
ATOM	4091	CG	PHE	B	1034	−12.171	38.935	43.234	1.00	28.49	B	C
ATOM	4092	CD1	PHE	B	1034	−11.569	38.664	42.009	1.00	25.37	B	C
ATOM	4093	CD2	PHE	B	1034	−12.770	40.178	43.423	1.00	26.16	B	C
ATOM	4094	CE1	PHE	B	1034	−11.564	39.612	40.996	1.00	25.58	B	C
ATOM	4095	CE2	PHE	B	1034	−12.764	41.129	42.407	1.00	26.17	B	C
ATOM	4096	CZ	PHE	B	1034	−12.160	40.842	41.194	1.00	25.18	B	C
ATOM	4097	C	PHE	B	1034	−12.594	37.620	46.785	1.00	26.89	B	C
ATOM	4098	O	PHE	B	1034	−13.633	37.991	47.324	1.00	26.48	B	O
ATOM	4099	N	LEU	B	1035	−11.986	36.483	47.091	1.00	29.42	B	N
ATOM	4100	CA	LEU	B	1035	−12.533	35.568	48.080	1.00	30.90	B	C
ATOM	4101	CB	LEU	B	1035	−11.767	34.243	48.025	1.00	30.10	B	C
ATOM	4102	CG	LEU	B	1035	−12.523	33.012	47.518	1.00	28.66	B	C
ATOM	4103	CD1	LEU	B	1035	−13.344	33.332	46.304	1.00	27.57	B	C
ATOM	4104	CD2	LEU	B	1035	−11.527	31.926	47.229	1.00	29.37	B	C

TABLE 2-continued

ATOM	4105	C	LEU	B	1035	−12.517	36.148	49.494	1.00	32.42	B	C
ATOM	4106	O	LEU	B	1035	−13.470	35.959	50.251	1.00	33.93	B	O
ATOM	4107	N	ARG	B	1036	−11.446	36.852	49.857	1.00	32.89	B	N
ATOM	4108	CA	ARG	B	1036	−11.380	37.443	51.189	1.00	34.45	B	C
ATOM	4109	CB	ARG	B	1036	−9.941	37.700	51.627	1.00	33.31	B	C
ATOM	4110	CG	ARG	B	1036	−9.195	38.666	50.758	1.00	35.78	B	C
ATOM	4111	CD	ARG	B	1036	−7.951	39.174	51.461	1.00	36.21	B	C
ATOM	4112	NE	ARG	B	1036	−8.294	40.190	52.447	1.00	34.88	B	N
ATOM	4113	CZ	ARG	B	1036	−8.240	41.498	52.220	1.00	33.46	B	C
ATOM	4114	NH1	ARG	B	1036	−7.850	41.955	51.040	1.00	33.99	B	N
ATOM	4115	NH2	ARG	B	1036	−8.589	42.352	53.169	1.00	34.43	B	N
ATOM	4116	C	ARG	B	1036	−12.163	38.743	51.250	1.00	35.70	B	C
ATOM	4117	O	ARG	B	1036	−12.517	39.196	52.333	1.00	37.83	B	O
ATOM	4118	N	MET	B	1037	−12.441	39.342	50.094	1.00	37.15	B	N
ATOM	4119	CA	MET	B	1037	−13.209	40.583	50.055	1.00	38.00	B	C
ATOM	4120	CB	MET	B	1037	−13.090	41.258	48.678	1.00	37.73	B	C
ATOM	4121	CG	MET	B	1037	−11.842	42.134	48.519	1.00	40.65	B	C
ATOM	4122	SD	MET	B	1037	−11.573	42.840	46.867	1.00	38.90	B	S
ATOM	4123	CE	MET	B	1037	−12.983	43.932	46.734	1.00	40.28	B	C
ATOM	4124	C	MET	B	1037	−14.680	40.331	50.389	1.00	39.11	B	C
ATOM	4125	O	MET	B	1037	−15.257	41.003	51.245	1.00	39.07	B	O
ATOM	4126	N	MET	B	1038	−15.292	39.357	49.728	1.00	41.37	B	N
ATOM	4127	CA	MET	B	1038	−16.697	39.072	49.991	1.00	43.13	B	C
ATOM	4128	CB	MET	B	1038	−17.395	38.660	48.692	1.00	43.22	B	C
ATOM	4129	CG	MET	B	1038	−16.556	37.788	47.794	1.00	43.58	B	C
ATOM	4130	SD	MET	B	1038	−17.231	37.655	46.142	1.00	41.45	B	S
ATOM	4131	CE	MET	B	1038	−18.295	36.342	46.357	1.00	41.55	B	C
ATOM	4132	C	MET	B	1038	−16.910	38.037	51.097	1.00	44.01	B	C
ATOM	4133	O	MET	B	1038	−18.017	37.543	51.301	1.00	44.45	B	O
ATOM	4134	N	GLY	B	1039	−15.834	37.739	51.820	1.00	46.15	B	N
ATOM	4135	CA	GLY	B	1039	−15.889	36.795	52.923	1.00	47.55	B	C
ATOM	4136	C	GLY	B	1039	−16.353	35.393	52.593	1.00	49.20	B	C
ATOM	4137	O	GLY	B	1039	−17.181	34.831	53.309	1.00	50.66	B	O
ATOM	4138	N	CYS	B	1040	−15.810	34.814	51.526	1.00	48.90	B	N
ATOM	4139	CA	CYS	B	1040	−16.198	33.471	51.119	1.00	47.27	B	C
ATOM	4140	CB	CYS	B	1040	−16.251	33.391	49.597	1.00	46.11	B	C
ATOM	4141	SG	CYS	B	1040	−16.885	31.828	48.977	1.00	45.49	B	S
ATOM	4142	C	CYS	B	1040	−15.242	32.411	51.655	1.00	47.59	B	C
ATOM	4143	O	CYS	B	1040	−14.040	32.468	51.405	1.00	46.95	B	O
ATOM	4144	N	GLU	B	1041	−15.780	31.445	52.395	1.00	48.51	B	N
ATOM	4145	CA	GLU	B	1041	−14.968	30.369	52.951	1.00	49.20	B	C
ATOM	4146	CB	GLU	B	1041	−15.517	29.926	54.317	1.00	48.69	B	C
ATOM	4147	CG	GLU	B	1041	−17.032	29.972	54.468	1.00	48.21	B	C
ATOM	4148	CD	GLU	B	1041	−17.513	29.317	55.764	1.00	48.81	B	C
ATOM	4149	OE1	GLU	B	1041	−18.715	29.444	56.080	1.00	47.24	B	O
ATOM	4150	OE2	GLU	B	1041	−16.691	28.670	56.461	1.00	48.13	B	O
ATOM	4151	C	GLU	B	1041	−14.894	29.186	51.986	1.00	49.69	B	C
ATOM	4152	O	GLU	B	1041	−14.219	28.186	52.243	1.00	49.89	B	O
ATOM	4153	N	ARG	B	1042	−15.598	29.315	50.868	1.00	50.29	B	N
ATOM	4154	CA	ARG	B	1042	−15.597	28.293	49.830	1.00	50.96	B	C
ATOM	4155	CB	ARG	B	1042	−16.953	28.251	49.123	1.00	52.40	B	C
ATOM	4156	CG	ARG	B	1042	−18.076	27.691	49.965	1.00	54.46	B	C
ATOM	4157	CD	ARG	B	1042	−19.371	27.654	49.179	1.00	56.84	B	C
ATOM	4158	NE	ARG	B	1042	−20.129	26.438	49.455	1.00	59.33	B	N
ATOM	4159	CZ	ARG	B	1042	−19.777	25.222	49.041	1.00	60.78	B	C
ATOM	4160	NH1	ARG	B	1042	−18.675	25.047	48.321	1.00	60.88	B	N
ATOM	4161	NH2	ARG	B	1042	−20.529	24.177	49.355	1.00	61.43	B	N
ATOM	4162	C	ARG	B	1042	−14.506	28.647	48.818	1.00	50.04	B	C
ATOM	4163	O	ARG	B	1042	−14.296	29.822	48.511	1.00	49.09	B	O
ATOM	4164	N	ASP	B	1043	−13.808	27.633	48.313	1.00	49.24	B	N
ATOM	4165	CA	ASP	B	1043	−12.747	27.846	47.336	1.00	46.56	B	C
ATOM	4166	CB	ASP	B	1043	−12.223	26.510	46.820	1.00	49.16	B	C
ATOM	4167	CG	ASP	B	1043	−11.444	25.747	47.864	1.00	52.26	B	C
ATOM	4168	OD1	ASP	B	1043	−10.478	26.327	48.401	1.00	52.24	B	O
ATOM	4169	OD2	ASP	B	1043	−11.793	24.571	48.135	1.00	53.66	B	O
ATOM	4170	C	ASP	B	1043	−13.247	28.673	46.160	1.00	43.96	B	C
ATOM	4171	O	ASP	B	1043	−12.509	29.483	45.609	1.00	43.39	B	O
ATOM	4172	N	VAL	B	1044	−14.496	28.448	45.768	1.00	42.85	B	N
ATOM	4173	CA	VAL	B	1044	−15.104	29.173	44.653	1.00	41.15	B	C
ATOM	4174	CB	VAL	B	1044	−15.403	28.255	43.436	1.00	38.53	B	C
ATOM	4175	CG1	VAL	B	1044	−16.208	29.008	42.390	1.00	37.89	B	C
ATOM	4176	CG2	VAL	B	1044	−14.120	27.781	42.821	1.00	38.24	B	C
ATOM	4177	C	VAL	B	1044	−16.416	29.743	45.143	1.00	40.47	B	C
ATOM	4178	O	VAL	B	1044	−17.240	29.034	45.701	1.00	40.60	B	O
ATOM	4179	N	PRO	B	1045	−16.621	31.042	44.938	1.00	40.56	B	N
ATOM	4180	CD	PRO	B	1045	−15.641	32.000	44.385	1.00	40.52	B	C
ATOM	4181	CA	PRO	B	1045	−17.843	31.719	45.362	1.00	40.24	B	C
ATOM	4182	CB	PRO	B	1045	−17.381	33.160	45.519	1.00	41.27	B	C
ATOM	4183	CG	PRO	B	1045	−16.426	33.307	44.352	1.00	40.98	B	C
ATOM	4184	C	PRO	B	1045	−18.935	31.597	44.318	1.00	39.56	B	C

TABLE 2-continued

ATOM	4185	O	PRO	B	1045	−18.665	31.260	43.173	1.00	39.45	B	O
ATOM	4186	N	ALA	B	1046	−20.170	31.868	44.725	1.00	40.46	B	N
ATOM	4187	CA	ALA	B	1046	−21.300	31.839	43.809	1.00	40.51	B	C
ATOM	4188	CB	ALA	B	1046	−22.600	32.073	44.568	1.00	40.27	B	C
ATOM	4189	C	ALA	B	1046	−21.038	32.989	42.838	1.00	40.45	B	C
ATOM	4190	O	ALA	B	1046	−20.504	34.029	43.235	1.00	39.83	B	O
ATOM	4191	N	LEU	B	1047	−21.403	32.807	41.574	1.00	39.65	B	N
ATOM	4192	CA	LEU	B	1047	−21.169	33.846	40.583	1.00	40.13	B	C
ATOM	4193	CB	LEU	B	1047	−21.357	33.289	39.162	1.00	40.46	B	C
ATOM	4194	CG	LEU	B	1047	−20.193	32.428	38.639	1.00	41.20	B	C
ATOM	4195	CD1	LEU	B	1047	−20.117	31.114	39.423	1.00	41.20	B	C
ATOM	4196	CD2	LEU	B	1047	−20.380	32.145	37.162	1.00	40.74	B	C
ATOM	4197	C	LEU	B	1047	−22.024	35.095	40.781	1.00	39.34	B	C
ATOM	4198	O	LEU	B	1047	−21.537	36.212	40.610	1.00	38.91	B	O
ATOM	4199	N	CYS	B	1048	−23.287	34.920	41.151	1.00	39.20	B	N
ATOM	4200	CA	CYS	B	1048	−24.162	36.068	41.363	1.00	39.30	B	C
ATOM	4201	CB	CYS	B	1048	−25.573	35.603	41.723	1.00	39.50	B	C
ATOM	4202	SG	CYS	B	1048	−25.664	34.837	43.349	1.00	42.73	B	S
ATOM	4203	C	CYS	B	1048	−23.600	36.928	42.495	1.00	39.35	B	C
ATOM	4204	O	CYS	B	1048	−23.779	38.145	42.519	1.00	39.73	B	O
ATOM	4205	N	ARG	B	1049	−22.916	36.282	43.432	1.00	38.09	B	N
ATOM	4206	CA	ARG	B	1049	−22.316	36.974	44.568	1.00	38.17	B	C
ATOM	4207	CB	ARG	B	1049	−21.897	35.931	45.600	1.00	40.51	B	C
ATOM	4208	CG	ARG	B	1049	−21.512	36.458	46.959	1.00	44.21	B	C
ATOM	4209	CD	ARG	B	1049	−21.091	35.286	47.845	1.00	48.40	B	C
ATOM	4210	NE	ARG	B	1049	−20.499	35.709	49.111	1.00	51.54	B	N
ATOM	4211	CZ	ARG	B	1049	−19.797	34.906	49.903	1.00	52.10	B	C
ATOM	4212	NH1	ARG	B	1049	−19.293	35.360	51.039	1.00	52.46	B	N
ATOM	4213	NH2	ARG	B	1049	−19.592	33.644	49.551	1.00	53.64	B	N
ATOM	4214	C	ARG	B	1049	−21.098	37.790	44.092	1.00	36.74	B	C
ATOM	4215	O	ARG	B	1049	−20.865	38.922	44.526	1.00	34.35	B	O
ATOM	4216	N	LEU	B	1050	−20.335	37.198	43.183	1.00	34.32	B	N
ATOM	4217	CA	LEU	B	1050	−19.152	37.840	42.630	1.00	33.57	B	C
ATOM	4218	CB	LEU	B	1050	−18.341	36.816	41.815	1.00	30.44	B	C
ATOM	4219	CG	LEU	B	1050	−17.161	37.394	41.031	1.00	29.65	B	C
ATOM	4220	CD1	LEU	B	1050	−16.365	38.366	41.921	1.00	26.93	B	C
ATOM	4221	CD2	LEU	B	1050	−16.306	36.283	40.494	1.00	22.80	B	C
ATOM	4222	C	LEU	B	1050	−19.563	39.028	41.753	1.00	33.51	B	C
ATOM	4223	O	LEU	B	1050	−18.971	40.105	41.835	1.00	32.04	B	O
ATOM	4224	N	LEU	B	1051	−20.581	38.817	40.920	1.00	34.24	B	N
ATOM	4225	CA	LEU	B	1051	−21.113	39.857	40.041	1.00	34.48	B	C
ATOM	4226	CB	LEU	B	1051	−22.277	39.287	39.216	1.00	34.57	B	C
ATOM	4227	CG	LEU	B	1051	−23.108	40.276	38.394	1.00	33.44	B	C
ATOM	4228	CD1	LEU	B	1051	−22.273	40.836	37.250	1.00	31.21	B	C
ATOM	4229	CD2	LEU	B	1051	−24.341	39.583	37.871	1.00	30.70	B	C
ATOM	4230	C	LEU	B	1051	−21.604	41.043	40.887	1.00	35.06	B	C
ATOM	4231	O	LEU	B	1051	−21.340	42.199	40.571	1.00	35.49	B	O
ATOM	4232	N	GLU	B	1052	−22.329	40.746	41.957	1.00	35.65	B	N
ATOM	4233	CA	GLU	B	1052	−22.837	41.781	42.848	1.00	37.17	B	C
ATOM	4234	CB	GLU	B	1052	−23.554	41.124	44.025	1.00	39.94	B	C
ATOM	4235	CG	GLU	B	1052	−24.094	42.072	45.076	1.00	42.75	B	C
ATOM	4236	CD	GLU	B	1052	−24.868	41.331	46.152	1.00	46.05	B	C
ATOM	4237	OE1	GLU	B	1052	−24.237	40.571	46.921	1.00	49.05	B	O
ATOM	4238	OE2	GLU	B	1052	−26.106	41.495	46.225	1.00	46.95	B	O
ATOM	4239	C	GLU	B	1052	−21.701	42.667	43.369	1.00	37.09	B	C
ATOM	4240	O	GLU	B	1052	−21.793	43.892	43.353	1.00	35.90	B	O
ATOM	4241	N	LEU	B	1053	−20.633	42.028	43.839	1.00	37.03	B	N
ATOM	4242	CA	LEU	B	1053	−19.476	42.735	44.371	1.00	34.66	B	C
ATOM	4243	CB	LEU	B	1053	−18.366	41.736	44.720	1.00	33.52	B	C
ATOM	4244	CG	LEU	B	1053	−17.020	42.336	45.133	1.00	33.63	B	C
ATOM	4245	CD1	LEU	B	1053	−17.136	42.940	46.515	1.00	32.45	B	C
ATOM	4246	CD2	LEU	B	1053	−15.945	41.268	45.100	1.00	34.11	B	C
ATOM	4247	C	LEU	B	1053	−18.970	43.734	43.340	1.00	34.06	B	C
ATOM	4248	O	LEU	B	1053	−18.637	44.868	43.678	1.00	33.84	B	O
ATOM	4249	N	LEU	B	1054	−18.913	43.303	42.083	1.00	33.58	B	N
ATOM	4250	CA	LEU	B	1054	−18.460	44.166	40.988	1.00	34.37	B	C
ATOM	4251	CB	LEU	B	1054	−18.126	43.323	39.747	1.00	33.25	B	C
ATOM	4252	CG	LEU	B	1054	−16.869	42.443	39.809	1.00	32.78	B	C
ATOM	4253	CD1	LEU	B	1054	−16.779	41.554	38.584	1.00	32.14	B	C
ATOM	4254	CD2	LEU	B	1054	−15.649	43.321	39.897	1.00	31.57	B	C
ATOM	4255	C	LEU	B	1054	−19.522	45.217	40.635	1.00	34.18	B	C
ATOM	4256	O	LEU	B	1054	−19.198	46.362	40.311	1.00	32.80	B	O
ATOM	4257	N	GLU	B	1055	−20.790	44.826	40.704	1.00	36.25	B	N
ATOM	4258	CA	GLU	B	1055	−21.877	45.748	40.396	1.00	38.15	B	C
ATOM	4259	CB	GLU	B	1055	−23.212	44.996	40.321	1.00	37.35	B	C
ATOM	4260	CG	GLU	B	1055	−23.379	44.222	39.022	1.00	40.80	B	C
ATOM	4261	CD	GLU	B	1055	−24.735	43.542	38.884	1.00	41.88	B	C
ATOM	4262	OE1	GLU	B	1055	−25.159	43.295	37.735	1.00	41.74	B	O
ATOM	4263	OE2	GLU	B	1055	−25.372	43.240	39.914	1.00	44.00	B	O
ATOM	4264	C	GLU	B	1055	−21.957	46.873	41.421	1.00	38.20	B	C

TABLE 2-continued

ATOM	4265	O	GLU	B	1055	−22.727	47.816	41.261	1.00	38.44	B	O
ATOM	4266	N	GLU	B	1056	−21.155	46.777	42.473	1.00	38.46	B	N
ATOM	4267	CA	GLU	B	1056	−21.156	47.811	43.490	1.00	39.89	B	C
ATOM	4268	CB	GLU	B	1056	−21.195	47.207	44.890	1.00	42.00	B	C
ATOM	4269	CG	GLU	B	1056	−22.401	46.326	45.151	1.00	47.57	B	C
ATOM	4270	CD	GLU	B	1056	−22.500	45.872	46.602	1.00	49.21	B	C
ATOM	4271	OE1	GLU	B	1056	−21.445	45.560	47.205	1.00	48.52	B	O
ATOM	4272	OE2	GLU	B	1056	−23.639	45.820	47.127	1.00	50.36	B	O
ATOM	4273	C	GLU	B	1056	−19.935	48.701	43.368	1.00	40.12	B	C
ATOM	4274	O	GLU	B	1056	−19.733	49.575	44.203	1.00	42.38	B	O
ATOM	4275	N	GLY	B	1057	−19.114	48.474	42.347	1.00	38.76	B	N
ATOM	4276	CA	GLY	B	1057	−17.934	49.302	42.155	1.00	36.47	B	C
ATOM	4277	C	GLY	B	1057	−16.638	48.773	42.739	1.00	36.71	B	C
ATOM	4278	O	GLY	B	1057	−15.565	49.343	42.521	1.00	37.03	B	O
ATOM	4279	N	GLN	B	1058	−16.728	47.677	43.481	1.00	35.24	B	N
ATOM	4280	CA	GLN	B	1058	−15.560	47.069	44.099	1.00	32.79	B	C
ATOM	4281	CB	GLN	B	1058	−16.011	45.969	45.057	1.00	32.99	B	C
ATOM	4282	CG	GLN	B	1058	−16.917	46.467	46.169	1.00	34.23	B	C
ATOM	4283	CD	GLN	B	1058	−16.242	46.452	47.527	1.00	34.06	B	C
ATOM	4284	OE1	GLN	B	1058	−15.024	46.622	47.630	1.00	34.44	B	O
ATOM	4285	NE2	GLN	B	1058	−17.035	46.262	48.581	1.00	31.51	B	N
ATOM	4286	C	GLN	B	1058	−14.588	46.487	43.072	1.00	33.29	B	C
ATOM	4287	O	GLN	B	1058	−14.984	45.704	42.209	1.00	34.91	B	O
ATOM	4288	N	ARG	B	1059	−13.317	46.872	43.174	1.00	32.14	B	N
ATOM	4289	CA	ARG	B	1059	−12.267	46.385	42.283	1.00	31.05	B	C
ATOM	4290	CB	ARG	B	1059	−11.729	47.519	41.417	1.00	31.00	B	C
ATOM	4291	CG	ARG	B	1059	−12.191	47.492	39.963	1.00	33.01	B	C
ATOM	4292	CD	ARG	B	1059	−13.652	47.142	39.862	1.00	32.34	B	C
ATOM	4293	NE	ARG	B	1059	−14.329	47.791	38.746	1.00	30.92	B	N
ATOM	4294	CZ	ARG	B	1059	−15.643	47.738	38.558	1.00	32.32	B	C
ATOM	4295	NH1	ARG	B	1059	−16.399	47.054	39.409	1.00	29.29	B	N
ATOM	4296	NH2	ARG	B	1059	−16.203	48.402	37.554	1.00	32.00	B	N
ATOM	4297	C	ARG	B	1059	−11.122	45.814	43.112	1.00	30.78	B	C
ATOM	4298	O	ARG	B	1059	−11.116	45.937	44.328	1.00	31.26	B	O
ATOM	4299	N	LEU	B	1060	−10.155	45.188	42.449	1.00	31.98	B	N
ATOM	4300	CA	LEU	B	1060	−8.999	44.620	43.131	1.00	32.82	B	C
ATOM	4301	CB	LEU	B	1060	−8.147	43.810	42.156	1.00	30.99	B	C
ATOM	4302	CG	LEU	B	1060	−8.791	42.576	41.510	1.00	33.63	B	C
ATOM	4303	CD1	LEU	B	1060	−7.897	42.047	40.385	1.00	32.89	B	C
ATOM	4304	CD2	LEU	B	1060	−9.035	41.513	42.570	1.00	30.44	B	C
ATOM	4305	C	LEU	B	1060	−8.137	45.719	43.731	1.00	35.16	B	C
ATOM	4306	O	LEU	B	1060	−8.011	46.808	43.165	1.00	35.31	B	O
ATOM	4307	N	PRO	B	1061	−7.526	45.448	44.891	1.00	37.66	B	N
ATOM	4308	CD	PRO	B	1061	−7.628	44.209	45.686	1.00	38.68	B	C
ATOM	4309	CA	PRO	B	1061	−6.666	46.429	45.557	1.00	38.74	B	C
ATOM	4310	CB	PRO	B	1061	−6.472	45.829	46.945	1.00	37.50	B	C
ATOM	4311	CG	PRO	B	1061	−6.461	44.351	46.661	1.00	39.71	B	C
ATOM	4312	C	PRO	B	1061	−5.355	46.560	44.798	1.00	40.11	B	C
ATOM	4313	O	PRO	B	1061	−4.671	45.566	44.570	1.00	42.72	B	O
ATOM	4314	N	ALA	B	1062	−5.023	47.787	44.406	1.00	40.89	B	N
ATOM	4315	CA	ALA	B	1062	−3.795	48.078	43.669	1.00	41.43	B	C
ATOM	4316	CB	ALA	B	1062	−3.455	49.565	43.791	1.00	42.02	B	C
ATOM	4317	C	ALA	B	1062	−2.620	47.242	44.162	1.00	40.81	B	C
ATOM	4318	O	ALA	B	1062	−2.380	47.136	45.365	1.00	40.36	B	O
ATOM	4319	N	PRO	B	1063	−1.874	46.629	43.230	1.00	40.11	B	N
ATOM	4320	CD	PRO	B	1063	−2.038	46.655	41.768	1.00	38.16	B	C
ATOM	4321	CA	PRO	B	1063	−0.727	45.810	43.619	1.00	40.35	B	C
ATOM	4322	CB	PRO	B	1063	−0.190	45.305	42.279	1.00	38.03	B	C
ATOM	4323	CG	PRO	B	1063	−0.667	46.318	41.298	1.00	36.80	B	C
ATOM	4324	C	PRO	B	1063	0.292	46.630	44.415	1.00	41.69	B	C
ATOM	4325	O	PRO	B	1063	0.612	47.763	44.052	1.00	40.07	B	O
ATOM	4326	N	PRO	B	1064	0.787	46.064	45.532	1.00	42.80	B	N
ATOM	4327	CD	PRO	B	1064	0.311	44.773	46.054	1.00	42.45	B	C
ATOM	4328	CA	PRO	B	1064	1.766	46.652	46.455	1.00	43.51	B	C
ATOM	4329	CB	PRO	B	1064	2.019	45.522	47.442	1.00	43.04	B	C
ATOM	4330	CG	PRO	B	1064	0.685	44.873	47.521	1.00	43.10	B	C
ATOM	4331	C	PRO	B	1064	3.051	47.123	45.798	1.00	43.88	B	C
ATOM	4332	O	PRO	B	1064	3.897	46.309	45.439	1.00	44.89	B	O
ATOM	4333	N	ALA	B	1065	3.182	48.437	45.639	1.00	43.57	B	N
ATOM	4334	CA	ALA	B	1065	4.363	49.047	45.033	1.00	44.73	B	C
ATOM	4335	CB	ALA	B	1065	5.617	48.244	45.384	1.00	44.54	B	C
ATOM	4336	C	ALA	B	1065	4.254	49.204	43.518	1.00	44.87	B	C
ATOM	4337	O	ALA	B	1065	5.240	49.491	42.840	1.00	45.51	B	O
ATOM	4338	N	CYS	B	1066	3.051	49.017	42.991	1.00	44.57	B	N
ATOM	4339	CA	CYS	B	1066	2.813	49.148	41.560	1.00	42.80	B	C
ATOM	4340	CB	CYS	B	1066	1.385	48.702	41.220	1.00	41.77	B	C
ATOM	4341	SG	CYS	B	1066	0.764	49.168	39.564	1.00	42.74	B	S
ATOM	4342	C	CYS	B	1066	2.999	50.582	41.111	1.00	41.34	B	C
ATOM	4343	O	CYS	B	1066	2.634	51.516	41.809	1.00	41.68	B	O
ATOM	4344	N	PRO	B	1067	3.599	50.774	39.941	1.00	40.50	B	N

TABLE 2-continued

ATOM	4345	CD	PRO	B	1067	4.318	49.776	39.135	1.00	40.21	B	C
ATOM	4346	CA	PRO	B	1067	3.803	52.123	39.423	1.00	40.36	B	C
ATOM	4347	CB	PRO	B	1067	4.405	51.863	38.054	1.00	39.69	B	C
ATOM	4348	CG	PRO	B	1067	5.223	50.636	38.290	1.00	38.76	B	C
ATOM	4349	C	PRO	B	1067	2.434	52.803	39.326	1.00	41.40	B	C
ATOM	4350	O	PRO	B	1067	1.429	52.153	39.022	1.00	42.80	B	O
ATOM	4351	N	ALA	B	1068	2.402	54.105	39.576	1.00	41.17	B	N
ATOM	4352	CA	ALA	B	1068	1.163	54.887	39.535	1.00	41.52	B	C
ATOM	4353	CB	ALA	B	1068	1.473	56.353	39.907	1.00	41.43	B	C
ATOM	4354	C	ALA	B	1068	0.383	54.829	38.203	1.00	40.64	B	C
ATOM	4355	O	ALA	B	1068	−0.825	54.584	38.192	1.00	39.24	B	O
ATOM	4356	N	GLU	B	1069	1.065	55.072	37.089	1.00	40.27	B	N
ATOM	4357	CA	GLU	B	1069	0.414	55.043	35.784	1.00	41.72	B	C
ATOM	4358	CB	GLU	B	1069	1.305	55.718	34.738	1.00	44.54	B	C
ATOM	4359	CG	GLU	B	1069	2.792	55.431	34.901	1.00	47.65	B	C
ATOM	4360	CD	GLU	B	1069	3.412	56.113	36.114	1.00	47.70	B	C
ATOM	4361	OE1	GLU	B	1069	3.262	57.343	36.252	1.00	47.97	B	O
ATOM	4362	OE2	GLU	B	1069	4.060	55.419	36.925	1.00	48.18	B	O
ATOM	4363	C	GLU	B	1069	0.040	53.627	35.332	1.00	41.70	B	C
ATOM	4364	O	GLU	B	1069	−0.907	53.441	34.562	1.00	41.28	B	O
ATOM	4365	N	VAL	B	1070	0.780	52.631	35.810	1.00	40.03	B	N
ATOM	4366	CA	VAL	B	1070	0.485	51.249	35.462	1.00	39.46	B	C
ATOM	4367	CB	VAL	B	1070	1.559	50.276	36.014	1.00	41.14	B	C
ATOM	4368	CG1	VAL	B	1070	0.924	48.927	36.330	1.00	41.59	B	C
ATOM	4369	CG2	VAL	B	1070	2.681	50.091	34.987	1.00	40.03	B	C
ATOM	4370	C	VAL	B	1070	−0.872	50.875	36.053	1.00	39.70	B	C
ATOM	4371	O	VAL	B	1070	−1.700	50.261	35.381	1.00	39.20	B	O
ATOM	4372	N	HIS	B	1071	−1.088	51.264	37.312	1.00	40.03	B	N
ATOM	4373	CA	HIS	B	1071	−2.331	50.994	38.041	1.00	40.05	B	C
ATOM	4374	CB	HIS	B	1071	−2.165	51.344	39.528	1.00	40.50	B	C
ATOM	4375	CG	HIS	B	1071	−3.399	51.124	40.349	1.00	41.67	B	C
ATOM	4376	CD2	HIS	B	1071	−4.059	51.943	41.203	1.00	40.99	B	C
ATOM	4377	ND1	HIS	B	1071	−4.090	49.932	40.358	1.00	42.50	B	N
ATOM	4378	CE1	HIS	B	1071	−5.123	50.025	41.177	1.00	38.81	B	C
ATOM	4379	NE2	HIS	B	1071	−5.125	51.235	41.701	1.00	39.78	B	N
ATOM	4380	C	HIS	B	1071	−3.488	51.794	37.462	1.00	40.65	B	C
ATOM	4381	O	HIS	B	1071	−4.645	51.403	37.587	1.00	40.56	B	O
ATOM	4382	N	GLU	B	1072	−3.178	52.919	36.829	1.00	40.18	B	N
ATOM	4383	CA	GLU	B	1072	−4.221	53.743	36.240	1.00	40.50	B	C
ATOM	4384	CB	GLU	B	1072	−3.693	55.157	35.975	1.00	44.39	B	C
ATOM	4385	CG	GLU	B	1072	−4.766	56.138	35.550	1.00	50.86	B	C
ATOM	4386	CD	GLU	B	1072	−4.385	57.579	35.834	1.00	55.90	B	C
ATOM	4387	OE1	GLU	B	1072	−3.348	58.034	35.303	1.00	57.49	B	O
ATOM	4388	OE2	GLU	B	1072	−5.122	58.253	36.593	1.00	58.81	B	O
ATOM	4389	C	GLU	B	1072	−4.735	53.102	34.947	1.00	38.98	B	C
ATOM	4390	O	GLU	B	1072	−5.900	53.263	34.588	1.00	37.76	B	O
ATOM	4391	N	LEU	B	1073	−3.870	52.367	34.249	1.00	37.52	B	N
ATOM	4392	CA	LEU	B	1073	−4.287	51.697	33.023	1.00	35.30	B	C
ATOM	4393	CB	LEU	B	1073	−3.090	51.114	32.267	1.00	34.93	B	C
ATOM	4394	CG	LEU	B	1073	−2.101	52.111	31.674	1.00	34.74	B	C
ATOM	4395	CD1	LEU	B	1073	−1.079	51.384	30.837	1.00	33.55	B	C
ATOM	4396	CD2	LEU	B	1073	−2.857	53.111	30.823	1.00	36.36	B	C
ATOM	4397	C	LEU	B	1073	−5.252	50.568	33.359	1.00	34.77	B	C
ATOM	4398	O	LEU	B	1073	−6.318	50.467	32.765	1.00	34.13	B	O
ATOM	4399	N	MET	B	1074	−4.878	49.719	34.313	1.00	35.06	B	N
ATOM	4400	CA	MET	B	1074	−5.742	48.608	34.690	1.00	33.81	B	C
ATOM	4401	CB	MET	B	1074	−5.022	47.632	35.632	1.00	32.66	B	C
ATOM	4402	CG	MET	B	1074	−4.646	48.183	36.999	1.00	30.09	B	C
ATOM	4403	SD	MET	B	1074	−3.884	46.950	38.130	1.00	23.51	B	S
ATOM	4404	CE	MET	B	1074	−2.271	46.878	37.495	1.00	21.36	B	C
ATOM	4405	C	MET	B	1074	−6.983	49.137	35.361	1.00	33.43	B	C
ATOM	4406	O	MET	B	1074	−7.960	48.422	35.516	1.00	35.76	B	O
ATOM	4407	N	LYS	B	1075	−6.956	50.401	35.748	1.00	32.86	B	N
ATOM	4408	CA	LYS	B	1075	−8.105	50.984	36.412	1.00	34.05	B	C
ATOM	4409	CB	LYS	B	1075	−7.717	52.305	37.081	1.00	36.76	B	C
ATOM	4410	CG	LYS	B	1075	−8.596	52.684	38.266	1.00	36.63	B	C
ATOM	4411	CD	LYS	B	1075	−8.189	51.893	39.498	1.00	36.73	B	C
ATOM	4412	CE	LYS	B	1075	−9.300	51.859	40.545	1.00	38.31	B	C
ATOM	4413	NZ	LYS	B	1075	−10.509	51.089	40.106	1.00	33.91	B	N
ATOM	4414	C	LYS	B	1075	−9.193	51.241	35.380	1.00	32.72	B	C
ATOM	4415	O	LYS	B	1075	−10.364	50.956	35.614	1.00	33.59	B	O
ATOM	4416	N	LEU	B	1076	−8.784	51.790	34.240	1.00	30.33	B	N
ATOM	4417	CA	LEU	B	1076	−9.687	52.113	33.143	1.00	27.87	B	C
ATOM	4418	CB	LEU	B	1076	−8.935	52.919	32.080	1.00	27.60	B	C
ATOM	4419	CG	LEU	B	1076	−8.395	54.307	32.467	1.00	25.81	B	C
ATOM	4420	CD1	LEU	B	1076	−7.729	54.956	31.266	1.00	23.58	B	C
ATOM	4421	CD2	LEU	B	1076	−9.539	55.179	32.947	1.00	23.87	B	C
ATOM	4422	C	LEU	B	1076	−10.263	50.853	32.511	1.00	27.92	B	C
ATOM	4423	O	LEU	B	1076	−11.416	50.818	32.067	1.00	27.92	B	O
ATOM	4424	N	CYS	B	1077	−9.437	49.818	32.466	1.00	25.91	B	N

TABLE 2-continued

ATOM	4425	CA	CYS	B	1077	−9.838	48.550	31.899	1.00	23.62	B	C
ATOM	4426	CB	CYS	B	1077	−8.695	47.538	32.002	1.00	21.19	B	C
ATOM	4427	SG	CYS	B	1077	−7.269	47.783	30.894	1.00	21.49	B	S
ATOM	4428	C	CYS	B	1077	−11.065	47.986	32.610	1.00	22.56	B	C
ATOM	4429	O	CYS	B	1077	−11.830	47.257	31.997	1.00	23.55	B	O
ATOM	4430	N	TRP	B	1078	−11.251	48.323	33.892	1.00	23.18	B	N
ATOM	4431	CA	TRP	B	1078	−12.374	47.797	34.684	1.00	21.44	B	C
ATOM	4432	CB	TRP	B	1078	−11.905	47.359	36.077	1.00	21.43	B	C
ATOM	4433	CG	TRP	B	1078	−10.755	46.398	36.077	1.00	23.00	B	C
ATOM	4434	CD2	TRP	B	1078	−9.714	46.318	37.054	1.00	23.77	B	C
ATOM	4435	CE2	TRP	B	1078	−8.834	45.293	36.647	1.00	24.28	B	C
ATOM	4436	CE3	TRP	B	1078	−9.438	47.017	38.233	1.00	22.51	B	C
ATOM	4437	CD1	TRP	B	1078	−10.478	45.437	35.145	1.00	26.11	B	C
ATOM	4438	NE1	TRP	B	1078	−9.322	44.772	35.478	1.00	25.75	B	N
ATOM	4439	CZ2	TRP	B	1078	−7.697	44.954	37.376	1.00	23.37	B	C
ATOM	4440	CZ3	TRP	B	1078	−8.314	46.679	38.950	1.00	22.43	B	C
ATOM	4441	CH2	TRP	B	1078	−7.455	45.656	38.520	1.00	22.90	B	C
ATOM	4442	C	TRP	B	1078	−13.592	48.712	34.831	1.00	20.28	B	C
ATOM	4443	O	TRP	B	1078	−14.348	48.621	35.798	1.00	15.97	B	O
ATOM	4444	N	ALA	B	1079	−13.772	49.593	33.860	1.00	21.94	B	N
ATOM	4445	CA	ALA	B	1079	−14.918	50.480	33.844	1.00	23.82	B	C
ATOM	4446	CB	ALA	B	1079	−14.838	51.408	32.645	1.00	21.74	B	C
ATOM	4447	C	ALA	B	1079	−16.138	49.569	33.726	1.00	26.53	B	C
ATOM	4448	O	ALA	B	1079	−16.111	48.555	33.027	1.00	26.44	B	O
ATOM	4449	N	PRO	B	1080	−17.221	49.918	34.417	1.00	28.40	B	N
ATOM	4450	CD	PRO	B	1080	−17.374	51.083	35.305	1.00	28.57	B	C
ATOM	4451	CA	PRO	B	1080	−18.441	49.113	34.374	1.00	29.60	B	C
ATOM	4452	CB	PRO	B	1080	−19.463	49.997	35.088	1.00	27.68	B	C
ATOM	4453	CG	PRO	B	1080	−18.624	50.737	36.086	1.00	27.42	B	C
ATOM	4454	C	PRO	B	1080	−18.876	48.741	32.954	1.00	30.91	B	C
ATOM	4455	O	PRO	B	1080	−18.977	47.556	32.625	1.00	33.35	B	O
ATOM	4456	N	SER	B	1081	−19.119	49.745	32.116	1.00	30.36	B	N
ATOM	4457	CA	SER	B	1081	−19.568	49.498	30.749	1.00	30.13	B	C
ATOM	4458	CB	SER	B	1081	−20.373	50.684	30.214	1.00	32.93	B	C
ATOM	4459	OG	SER	B	1081	−19.514	51.762	29.886	1.00	37.08	B	O
ATOM	4460	C	SER	B	1081	−18.422	49.223	29.799	1.00	28.16	B	C
ATOM	4461	O	SER	B	1081	−17.355	49.822	29.894	1.00	28.59	B	O
ATOM	4462	N	PRO	B	1082	−18.643	48.313	28.849	1.00	26.55	B	N
ATOM	4463	CD	PRO	B	1082	−19.807	47.418	28.779	1.00	23.40	B	C
ATOM	4464	CA	PRO	B	1082	−17.633	47.938	27.861	1.00	26.35	B	C
ATOM	4465	CB	PRO	B	1082	−18.315	46.807	27.103	1.00	23.94	B	C
ATOM	4466	CG	PRO	B	1082	−19.214	46.207	28.152	1.00	22.82	B	C
ATOM	4467	C	PRO	B	1082	−17.209	49.097	26.954	1.00	28.24	B	C
ATOM	4468	O	PRO	B	1082	−16.021	49.294	26.681	1.00	27.35	B	O
ATOM	4469	N	GLN	B	1083	−18.184	49.866	26.493	1.00	28.90	B	N
ATOM	4470	CA	GLN	B	1083	−17.897	50.992	25.629	1.00	32.63	B	C
ATOM	4471	CB	GLN	B	1083	−19.208	51.615	25.163	1.00	36.33	B	C
ATOM	4472	CG	GLN	B	1083	−20.063	52.140	26.290	1.00	44.10	B	C
ATOM	4473	CD	GLN	B	1083	−21.349	52.781	25.796	1.00	47.98	B	C
ATOM	4474	OE1	GLN	B	1083	−22.121	52.160	25.059	1.00	50.30	B	O
ATOM	4475	NE2	GLN	B	1083	−21.592	54.029	26.208	1.00	50.00	B	N
ATOM	4476	C	GLN	B	1083	−17.012	52.050	26.318	1.00	33.60	B	C
ATOM	4477	O	GLN	B	1083	−16.493	52.961	25.669	1.00	33.23	B	O
ATOM	4478	N	ASP	B	1084	−16.821	51.926	27.626	1.00	34.03	B	N
ATOM	4479	CA	ASP	B	1084	−15.999	52.895	28.341	1.00	35.82	B	C
ATOM	4480	CB	ASP	B	1084	−16.627	53.227	29.704	1.00	38.13	B	C
ATOM	4481	CG	ASP	B	1084	−17.865	54.113	29.579	1.00	38.77	B	C
ATOM	4482	OD1	ASP	B	1084	−18.596	54.275	30.580	1.00	40.28	B	O
ATOM	4483	OD2	ASP	B	1084	−18.102	54.655	28.479	1.00	40.01	B	O
ATOM	4484	C	ASP	B	1084	−14.549	52.438	28.521	1.00	35.43	B	C
ATOM	4485	O	ASP	B	1084	−13.646	53.262	28.708	1.00	34.85	B	O
ATOM	4486	N	ARG	B	1085	−14.325	51.129	28.460	1.00	33.57	B	N
ATOM	4487	CA	ARG	B	1085	−12.980	50.589	28.603	1.00	31.02	B	C
ATOM	4488	CB	ARG	B	1085	−13.025	49.064	28.690	1.00	27.37	B	C
ATOM	4489	CG	ARG	B	1085	−13.849	48.558	29.856	1.00	25.02	B	C
ATOM	4490	CD	ARG	B	1085	−14.021	47.069	29.809	1.00	22.29	B	C
ATOM	4491	NE	ARG	B	1085	−15.125	46.671	30.665	1.00	21.69	B	N
ATOM	4492	CZ	ARG	B	1085	−15.985	45.702	30.374	1.00	20.52	B	C
ATOM	4493	NH1	ARG	B	1085	−15.873	45.015	29.246	1.00	17.94	B	N
ATOM	4494	NH2	ARG	B	1085	−16.975	45.438	31.210	1.00	20.52	B	N
ATOM	4495	C	ARG	B	1085	−12.194	51.012	27.375	1.00	30.75	B	C
ATOM	4496	O	ARG	B	1085	−12.742	51.116	26.289	1.00	32.84	B	O
ATOM	4497	N	PRO	B	1086	−10.897	51.280	27.532	1.00	30.76	B	N
ATOM	4498	CD	PRO	B	1086	−10.048	51.250	28.734	1.00	29.24	B	C
ATOM	4499	CA	PRO	B	1086	−10.132	51.688	26.355	1.00	30.29	B	C
ATOM	4500	CB	PRO	B	1086	−8.802	52.147	26.950	1.00	29.66	B	C
ATOM	4501	CG	PRO	B	1086	−8.654	51.273	28.137	1.00	29.74	B	C
ATOM	4502	C	PRO	B	1086	−9.971	50.509	25.421	1.00	29.51	B	C
ATOM	4503	O	PRO	B	1086	−10.398	49.407	25.732	1.00	32.54	B	O
ATOM	4504	N	SER	B	1087	−9.364	50.742	24.270	1.00	29.78	B	N

TABLE 2-continued

ATOM	4505	CA	SER	B	1087	−9.141	49.668	23.325	1.00	29.49	B	C
ATOM	4506	CB	SER	B	1087	−9.447	50.139	21.906	1.00	26.96	B	C
ATOM	4507	OG	SER	B	1087	−8.416	50.983	21.422	1.00	30.79	B	O
ATOM	4508	C	SER	B	1087	−7.664	49.300	23.439	1.00	29.09	B	C
ATOM	4509	O	SER	B	1087	−6.864	50.087	23.936	1.00	30.95	B	O
ATOM	4510	N	PHE	B	1088	−7.303	48.108	22.987	1.00	28.19	B	N
ATOM	4511	CA	PHE	B	1088	−5.919	47.679	23.038	1.00	27.93	B	C
ATOM	4512	CB	PHE	B	1088	−5.809	46.252	22.509	1.00	26.98	B	C
ATOM	4513	CG	PHE	B	1088	−6.217	45.204	23.510	1.00	26.32	B	C
ATOM	4514	CD1	PHE	B	1088	−5.428	44.957	24.627	1.00	23.88	B	C
ATOM	4515	CD2	PHE	B	1088	−7.384	44.466	23.336	1.00	23.74	B	C
ATOM	4516	CE1	PHE	B	1088	−5.793	43.997	25.545	1.00	23.97	B	C
ATOM	4517	CE2	PHE	B	1088	−7.757	43.500	24.257	1.00	23.15	B	C
ATOM	4518	CZ	PHE	B	1088	−6.961	43.264	25.362	1.00	24.05	B	C
ATOM	4519	C	PHE	B	1088	−5.037	48.622	22.226	1.00	29.08	B	C
ATOM	4520	O	PHE	B	1088	−3.855	48.786	22.517	1.00	30.69	B	O
ATOM	4521	N	SER	B	1089	−5.619	49.253	21.213	1.00	29.50	B	N
ATOM	4522	CA	SER	B	1089	−4.867	50.177	20.381	1.00	31.30	B	C
ATOM	4523	CB	SER	B	1089	−5.679	50.555	19.143	1.00	31.23	B	C
ATOM	4524	OG	SER	B	1089	−6.889	51.188	19.509	1.00	34.90	B	O
ATOM	4525	C	SER	B	1089	−4.530	51.427	21.190	1.00	32.13	B	C
ATOM	4526	O	SER	B	1089	−3.568	52.140	20.880	1.00	30.23	B	O
ATOM	4527	N	ALA	B	1090	−5.337	51.678	22.221	1.00	31.60	B	N
ATOM	4528	CA	ALA	B	1090	−5.138	52.816	23.107	1.00	33.02	B	C
ATOM	4529	CB	ALA	B	1090	−6.446	53.174	23.792	1.00	32.78	B	C
ATOM	4530	C	ALA	B	1090	−4.064	52.521	24.157	1.00	33.92	B	C
ATOM	4531	O	ALA	B	1090	−3.083	53.262	24.286	1.00	34.82	B	O
ATOM	4532	N	LEU	B	1091	−4.241	51.430	24.895	1.00	33.05	B	N
ATOM	4533	CA	LEU	B	1091	−3.284	51.053	25.929	1.00	32.35	B	C
ATOM	4534	CB	LEU	B	1091	−3.745	49.772	26.618	1.00	30.82	B	C
ATOM	4535	CG	LEU	B	1091	−5.128	49.884	27.254	1.00	29.77	B	C
ATOM	4536	CD1	LEU	B	1091	−5.770	48.510	27.366	1.00	27.39	B	C
ATOM	4537	CD2	LEU	B	1091	−4.999	50.558	28.605	1.00	31.11	B	C
ATOM	4538	C	LEU	B	1091	−1.879	50.858	25.366	1.00	32.88	B	C
ATOM	4539	O	LEU	B	1091	−0.893	51.290	25.974	1.00	32.53	B	O
ATOM	4540	N	GLY	B	1092	−1.807	50.208	24.204	1.00	32.64	B	N
ATOM	4541	CA	GLY	B	1092	−0.540	49.928	23.538	1.00	32.84	B	C
ATOM	4542	C	GLY	B	1092	0.515	51.017	23.583	1.00	32.38	B	C
ATOM	4543	O	GLY	B	1092	1.548	50.839	24.215	1.00	30.96	B	O
ATOM	4544	N	PRO	B	1093	0.293	52.152	22.904	1.00	34.39	B	N
ATOM	4545	CD	PRO	B	1093	−0.890	52.468	22.089	1.00	35.39	B	C
ATOM	4546	CA	PRO	B	1093	1.239	53.269	22.881	1.00	36.18	B	C
ATOM	4547	CB	PRO	B	1093	0.530	54.305	22.000	1.00	36.68	B	C
ATOM	4548	CG	PRO	B	1093	−0.915	53.969	22.159	1.00	35.69	B	C
ATOM	4549	C	PRO	B	1093	1.557	53.779	24.284	1.00	35.73	B	C
ATOM	4550	O	PRO	B	1093	2.705	54.093	24.583	1.00	34.76	B	O
ATOM	4551	N	GLN	B	1094	0.547	53.852	25.146	1.00	37.32	B	N
ATOM	4552	CA	GLN	B	1094	0.783	54.301	26.516	1.00	39.11	B	C
ATOM	4553	CB	GLN	B	1094	−0.526	54.389	27.309	1.00	39.49	B	C
ATOM	4554	CG	GLN	B	1094	−1.545	55.394	26.781	1.00	43.75	B	C
ATOM	4555	CD	GLN	B	1094	−2.660	55.693	27.789	1.00	47.08	B	C
ATOM	4556	OE1	GLN	B	1094	−2.397	56.218	28.874	1.00	49.17	B	O
ATOM	4557	NE2	GLN	B	1094	−3.903	55.362	27.434	1.00	46.08	B	N
ATOM	4558	C	GLN	B	1094	1.740	53.335	27.222	1.00	39.18	B	C
ATOM	4559	O	GLN	B	1094	2.728	53.758	27.817	1.00	40.18	B	O
ATOM	4560	N	LEU	B	1095	1.452	52.038	27.154	1.00	39.55	B	N
ATOM	4561	CA	LEU	B	1095	2.312	51.045	27.793	1.00	40.38	B	C
ATOM	4562	CB	LEU	B	1095	1.740	49.637	27.607	1.00	38.68	B	C
ATOM	4563	CG	LEU	B	1095	0.575	49.259	28.533	1.00	39.13	B	C
ATOM	4564	CD1	LEU	B	1095	−0.133	48.024	28.010	1.00	37.02	B	C
ATOM	4565	CD2	LEU	B	1095	1.104	49.031	29.943	1.00	37.97	B	C
ATOM	4566	C	LEU	B	1095	3.741	51.087	27.257	1.00	41.75	B	C
ATOM	4567	O	LEU	B	1095	4.704	51.027	28.023	1.00	40.09	B	O
ATOM	4568	N	ASP	B	1096	3.879	51.192	25.941	1.00	43.20	B	N
ATOM	4569	CA	ASP	B	1096	5.199	51.229	25.336	1.00	45.21	B	C
ATOM	4570	CB	ASP	B	1096	5.086	51.289	23.814	1.00	47.28	B	C
ATOM	4571	CG	ASP	B	1096	6.277	50.658	23.127	1.00	50.41	B	C
ATOM	4572	OD1	ASP	B	1096	7.018	51.376	22.411	1.00	51.05	B	O
ATOM	4573	OD2	ASP	B	1096	6.471	49.434	23.317	1.00	51.68	B	O
ATOM	4574	C	ASP	B	1096	5.969	52.432	25.857	1.00	44.84	B	C
ATOM	4575	O	ASP	B	1096	7.188	52.389	26.014	1.00	43.07	B	O
ATOM	4576	N	MET	B	1097	5.240	53.506	26.132	1.00	46.20	B	N
ATOM	4577	CA	MET	B	1097	5.839	54.722	26.655	1.00	47.53	B	C
ATOM	4578	CB	MET	B	1097	4.805	55.845	26.679	1.00	50.08	B	C
ATOM	4579	CG	MET	B	1097	5.362	57.174	27.161	1.00	53.76	B	C
ATOM	4580	SD	MET	B	1097	4.083	58.421	27.455	1.00	59.09	B	S
ATOM	4581	CE	MET	B	1097	3.697	58.094	29.210	1.00	56.01	B	C
ATOM	4582	C	MET	B	1097	6.378	54.482	28.069	1.00	47.41	B	C
ATOM	4583	O	MET	B	1097	7.551	54.746	28.346	1.00	47.55	B	O
ATOM	4584	N	LEU	B	1098	5.524	53.979	28.960	1.00	45.95	B	N

TABLE 2-continued

ATOM	4585	CA	LEU	B	1098	5.934	53.703	30.340	1.00	46.87	B	C
ATOM	4586	CB	LEU	B	1098	4.808	53.000	31.109	1.00	45.75	B	C
ATOM	4587	CG	LEU	B	1098	3.507	53.792	31.244	1.00	45.44	B	C
ATOM	4588	CD1	LEU	B	1098	2.490	53.006	32.075	1.00	45.54	B	C
ATOM	4589	CD2	LEU	B	1098	3.809	55.143	31.891	1.00	45.95	B	C
ATOM	4590	C	LEU	B	1098	7.195	52.841	30.395	1.00	47.11	B	C
ATOM	4591	O	LEU	B	1098	8.103	53.096	31.188	1.00	48.02	B	O
ATOM	4592	N	TRP	B	1099	7.240	51.821	29.547	1.00	47.69	B	N
ATOM	4593	CA	TRP	B	1099	8.380	50.920	29.480	1.00	48.25	B	C
ATOM	4594	CB	TRP	B	1099	8.231	49.990	28.279	1.00	47.18	B	C
ATOM	4595	CG	TRP	B	1099	9.403	49.114	28.085	1.00	45.90	B	C
ATOM	4596	CD2	TRP	B	1099	10.442	49.287	27.124	1.00	46.24	B	C
ATOM	4597	CE2	TRP	B	1099	11.365	48.244	27.319	1.00	46.53	B	C
ATOM	4598	CE3	TRP	B	1099	10.689	50.229	26.126	1.00	46.72	B	C
ATOM	4599	CD1	TRP	B	1099	9.720	48.004	28.800	1.00	46.60	B	C
ATOM	4600	NE1	TRP	B	1099	10.899	47.469	28.346	1.00	45.86	B	N
ATOM	4601	CZ2	TRP	B	1099	12.508	48.110	26.541	1.00	47.39	B	C
ATOM	4602	CZ3	TRP	B	1099	11.825	50.095	25.356	1.00	46.84	B	C
ATOM	4603	CH2	TRP	B	1099	12.723	49.047	25.570	1.00	47.41	B	C
ATOM	4604	C	TRP	B	1099	9.682	51.707	29.361	1.00	49.00	B	C
ATOM	4605	O	TRP	B	1099	10.600	51.531	30.160	1.00	48.96	B	O
ATOM	4606	N	SER	B	1100	9.757	52.575	28.358	1.00	49.38	B	N
ATOM	4607	CA	SER	B	1100	10.943	53.395	28.149	1.00	50.99	B	C
ATOM	4608	CB	SER	B	1100	10.966	53.916	26.714	1.00	50.66	B	C
ATOM	4609	OG	SER	B	1100	9.892	54.814	26.492	1.00	50.60	B	O
ATOM	4610	C	SER	B	1100	10.975	54.579	29.128	1.00	51.72	B	C
ATOM	4611	O	SER	B	1100	11.903	54.640	29.961	1.00	52.69	B	O
ATOM	4612	OXT	SER	B	1100	10.071	55.437	29.060	1.00	52.10	B	O
TER	1		SER	B	1100						B	
HETATM	4625	P1	AMP	Y	1	26.248	46.926	4.305	1.00	28.91	Y	P
HETATM	4626	O1	AMP	Y	1	24.959	46.349	4.017	1.00	29.03	Y	O
HETATM	4627	O2	AMP	Y	1	26.471	48.087	3.460	1.00	23.13	Y	O
HETATM	4628	O3	AMP	Y	1	27.346	45.981	4.135	1.00	27.39	Y	O
HETATM	4629	P2	AMP	Y	1	25.260	48.053	6.796	1.00	28.00	Y	P
HETATM	4630	O4	AMP	Y	1	24.100	47.197	6.818	1.00	27.56	Y	O
HETATM	4631	O5	AMP	Y	1	25.860	48.106	8.087	1.00	27.82	Y	O
HETATM	4632	N2	AMP	Y	1	26.211	47.226	5.864	1.00	28.12	Y	N
HETATM	4633	P3	AMP	Y	1	23.678	50.169	5.602	1.00	24.33	Y	P
HETATM	4634	O6	AMP	Y	1	24.107	51.460	4.951	1.00	28.59	Y	O
HETATM	4635	O7	AMP	Y	1	23.048	49.307	4.652	1.00	25.29	Y	O
HETATM	4636	O8	AMP	Y	1	25.027	49.513	6.240	1.00	26.20	Y	O
HETATM	4637	O9	AMP	Y	1	22.642	50.469	6.693	1.00	23.79	Y	O
HETATM	4638	C1	AMP	Y	1	22.965	51.477	7.584	1.00	22.50	Y	C
HETATM	4639	C3	AMP	Y	1	22.381	51.189	8.968	1.00	23.70	Y	C
HETATM	4640	O10	AMP	Y	1	20.972	51.326	8.978	1.00	22.51	Y	O
HETATM	4641	C7	AMP	Y	1	22.646	49.806	9.574	1.00	23.88	Y	C
HETATM	4642	O11	AMP	Y	1	22.712	49.938	10.970	1.00	27.97	Y	O
HETATM	4643	C9	AMP	Y	1	21.390	49.035	9.243	1.00	23.07	Y	C
HETATM	4644	O12	AMP	Y	1	21.146	48.025	10.175	1.00	20.17	Y	O
HETATM	4645	C10	AMP	Y	1	20.313	50.104	9.309	1.00	22.71	Y	C
HETATM	4646	N4	AMP	Y	1	19.162	49.846	8.397	1.00	23.97	Y	N
HETATM	4647	C8	AMP	Y	1	19.211	49.660	7.018	1.00	23.33	Y	C
HETATM	4648	N5	AMP	Y	1	17.986	49.386	6.524	1.00	23.11	Y	N
HETATM	4649	C5	AMP	Y	1	17.127	49.389	7.573	1.00	23.16	Y	C
HETATM	4650	C6	AMP	Y	1	15.741	49.186	7.842	1.00	23.60	Y	C
HETATM	4651	N6	AMP	Y	1	14.807	48.895	6.873	1.00	22.95	Y	N
HETATM	4652	N1	AMP	Y	1	15.244	49.269	9.124	1.00	26.75	Y	N
HETATM	4653	C2	AMP	Y	1	15.984	49.546	10.260	1.00	22.61	Y	C
HETATM	4654	N3	AMP	Y	1	17.313	49.758	10.097	1.00	23.12	Y	N
HETATM	4655	C4	AMP	Y	1	17.889	49.687	8.808	1.00	23.32	Y	C
HETATM	4656	MG	MG	Y	2	22.965	47.144	4.708	1.00	27.65	Y	MG
HETATM	4657	P1	AMP	Z	1	−6.811	27.348	31.249	1.00	29.75	Z	P
HETATM	4658	O1	AMP	Z	1	−6.300	27.933	30.032	1.00	25.93	Z	O
HETATM	4659	O2	AMP	Z	1	−7.551	26.124	30.969	1.00	24.41	Z	O
HETATM	4660	O3	AMP	Z	1	−7.613	28.224	32.090	1.00	26.59	Z	O
HETATM	4661	P2	AMP	Z	1	−4.222	26.039	31.829	1.00	26.40	Z	P
HETATM	4662	O4	AMP	Z	1	−3.371	26.742	30.880	1.00	26.33	Z	O
HETATM	4663	O5	AMP	Z	1	−3.594	25.914	33.084	1.00	27.90	Z	O
HETATM	4664	N2	AMP	Z	1	−5.480	27.010	32.143	1.00	28.13	Z	N
HETATM	4665	P3	AMP	Z	1	−4.457	23.966	29.840	1.00	26.27	Z	P
HETATM	4666	O6	AMP	Z	1	−5.338	22.775	29.725	1.00	28.28	Z	O
HETATM	4667	O7	AMP	Z	1	−4.637	24.880	28.724	1.00	27.16	Z	O
HETATM	4668	O8	AMP	Z	1	−4.755	24.626	31.283	1.00	25.90	Z	O
HETATM	4669	O9	AMP	Z	1	−2.951	23.529	29.790	1.00	25.56	Z	O
HETATM	4670	C1	AMP	Z	1	−2.309	22.819	30.848	1.00	22.33	Z	C
HETATM	4671	C3	AMP	Z	1	−0.795	23.071	30.857	1.00	23.34	Z	C
HETATM	4672	O10	AMP	Z	1	−0.234	22.965	29.547	1.00	22.37	Z	O
HETATM	4673	C7	AMP	Z	1	−0.408	24.496	31.335	1.00	23.19	Z	C
HETATM	4674	O11	AMP	Z	1	0.745	24.342	32.105	1.00	25.77	Z	O
HETATM	4675	C9	AMP	Z	1	−0.090	25.231	30.042	1.00	22.68	Z	C

TABLE 2-continued

HETATM	4676	O12	AMP	Z	1	0.844	26.255	30.179	1.00	22.55	Z	O
HETATM	4677	C10	AMP	Z	1	0.452	24.151	29.138	1.00	22.80	Z	C
HETATM	4678	N4	AMP	Z	1	0.396	24.436	27.666	1.00	24.01	Z	N
HETATM	4679	C8	AMP	Z	1	−0.742	24.730	26.933	1.00	24.62	Z	C
HETATM	4680	N5	AMP	Z	1	−0.447	24.966	25.604	1.00	25.25	Z	N
HETATM	4681	C5	AMP	Z	1	0.891	24.823	25.461	1.00	24.14	Z	C
HETATM	4682	C6	AMP	Z	1	1.915	24.885	24.448	1.00	24.17	Z	C
HETATM	4683	N6	AMP	Z	1	1.681	25.214	23.143	1.00	20.34	Z	N
HETATM	4684	N1	AMP	Z	1	3.266	24.622	24.771	1.00	25.74	Z	N
HETATM	4685	C2	AMP	Z	1	3.694	24.311	26.030	1.00	22.91	Z	C
HETATM	4686	N3	AMP	Z	1	2.771	24.244	27.043	1.00	21.55	Z	N
HETATM	4687	C4	AMP	Z	1	1.437	24.478	26.810	1.00	22.73	Z	C
HETATM	4688	MG	MG	Z	2	−4.549	27.191	28.573	1.00	31.30	Z	MG
HETATM	4689	O	HOH	W	1	−2.475	30.329	15.504	1.00	11.40	W	O
HETATM	4690	O	HOH	W	2	12.414	45.490	15.244	1.00	13.21	W	O
HETATM	4691	O	HOH	W	3	29.299	47.960	7.015	1.00	20.72	W	O
HETATM	4692	O	HOH	W	4	−8.081	23.906	29.636	1.00	24.82	W	O
HETATM	4693	O	HOH	W	5	19.546	44.643	17.339	1.00	5.81	W	O
HETATM	4694	O	HOH	W	6	−5.932	29.329	7.200	1.00	26.30	W	O
HETATM	4695	O	HOH	W	7	13.335	45.024	29.684	1.00	26.89	W	O
HETATM	4696	O	HOH	W	8	−2.722	34.331	39.767	1.00	28.35	W	O
HETATM	4697	O	HOH	W	9	35.150	40.728	−7.044	1.00	32.32	W	O
HETATM	4698	O	HOH	W	10	−21.199	33.084	32.518	1.00	29.13	W	O
HETATM	4699	O	HOH	W	11	1.946	41.700	15.699	1.00	17.00	W	O
HETATM	4700	O	HOH	W	12	−4.135	15.706	24.394	1.00	26.37	W	O
HETATM	4701	O	HOH	W	13	18.978	58.280	2.913	1.00	29.75	W	O
HETATM	4702	O	HOH	W	14	24.050	58.118	8.115	1.00	33.81	W	O
HETATM	4703	O	HOH	W	15	8.875	64.811	12.194	1.00	32.66	W	O
HETATM	4704	O	HOH	W	16	48.673	31.147	15.865	1.00	19.28	W	O
HETATM	4705	O	HOH	W	17	51.031	42.556	6.078	1.00	39.02	W	O
HETATM	4706	O	HOH	W	18	25.398	50.597	2.357	1.00	20.20	W	O
HETATM	4707	O	HOH	W	19	40.324	26.361	16.008	1.00	27.85	W	O
HETATM	4708	O	HOH	W	20	33.653	51.255	1.318	1.00	24.99	W	O
HETATM	4709	O	HOH	W	21	28.596	48.674	9.568	1.00	27.69	W	O
HETATM	4710	O	HOH	W	22	3.864	6.537	26.814	1.00	30.27	W	O
HETATM	4711	O	HOH	W	23	34.593	52.731	−2.102	1.00	21.01	W	O
HETATM	4712	O	HOH	W	24	3.459	12.452	32.479	1.00	16.68	W	O
HETATM	4713	O	HOH	W	25	21.173	61.854	13.602	1.00	18.35	W	O
HETATM	4714	O	HOH	W	26	−9.899	40.661	21.126	1.00	14.79	W	O
HETATM	4715	O	HOH	W	27	−6.606	26.300	34.986	1.00	26.71	W	O
HETATM	4716	O	HOH	W	28	31.882	37.812	13.934	1.00	24.97	W	O
HETATM	4717	O	HOH	W	29	5.767	35.379	−5.080	1.00	26.68	W	O
HETATM	4718	O	HOH	W	30	−0.387	12.747	10.060	1.00	30.83	W	O
HETATM	4719	O	HOH	W	31	−2.871	16.142	31.823	1.00	27.26	W	O
HETATM	4720	O	HOH	W	32	−11.338	17.892	21.567	1.00	24.99	W	O
HETATM	4721	O	HOH	W	33	27.741	41.030	9.385	1.00	35.57	W	O
HETATM	4722	O	HOH	W	34	4.219	40.947	15.023	1.00	26.11	W	O
HETATM	4723	O	HOH	W	35	13.358	40.025	45.175	1.00	33.41	W	O
HETATM	4724	O	HOH	W	36	10.178	43.642	−0.473	1.00	21.44	W	O
HETATM	4725	O	HOH	W	37	−5.670	25.835	23.800	1.00	26.16	W	O
HETATM	4726	O	HOH	W	38	22.553	65.325	10.636	1.00	35.15	W	O
HETATM	4727	O	HOH	W	39	−19.914	17.680	11.168	1.00	22.16	W	O
HETATM	4728	O	HOH	W	40	14.142	46.495	2.450	1.00	24.14	W	O
HETATM	4729	O	HOH	W	41	30.519	39.861	12.539	1.00	36.50	W	O
HETATM	4730	O	HOH	W	42	19.597	33.906	−3.688	1.00	17.47	W	O
HETATM	4731	O	HOH	W	43	16.289	45.356	3.477	1.00	17.51	W	O
HETATM	4732	O	HOH	W	44	21.782	43.355	−2.963	1.00	20.88	W	O
HETATM	4733	O	HOH	W	45	−8.473	49.357	41.780	1.00	25.18	W	O
HETATM	4734	O	HOH	W	46	−14.467	25.593	49.502	1.00	36.38	W	O
HETATM	4735	O	HOH	W	47	2.639	57.400	5.791	1.00	28.77	W	O
HETATM	4736	O	HOH	W	48	9.875	15.041	10.250	1.00	39.43	W	O
HETATM	4737	O	HOH	W	49	12.865	4.298	11.454	1.00	42.78	W	O
HETATM	4738	O	HOH	W	50	−18.417	36.077	56.375	1.00	34.15	W	O
HETATM	4739	O	HOH	W	51	−1.916	27.652	19.935	1.00	22.92	W	O
HETATM	4740	O	HOH	W	52	7.220	17.804	12.275	1.00	44.35	W	O
HETATM	4741	O	HOH	W	53	48.699	45.704	12.632	1.00	30.47	W	O
HETATM	4742	O	HOH	W	54	−2.981	8.858	20.070	1.00	23.68	W	O
HETATM	4743	O	HOH	W	55	−4.013	26.398	36.017	1.00	22.25	W	O
HETATM	4744	O	HOH	W	56	40.677	24.839	−3.765	1.00	25.15	W	O
HETATM	4745	O	HOH	W	57	−20.509	33.232	20.262	1.00	42.21	W	O
HETATM	4746	O	HOH	W	58	18.916	63.958	14.464	1.00	33.09	W	O
HETATM	4747	O	HOH	W	59	6.936	41.796	15.875	1.00	31.02	W	O
HETATM	4748	O	HOH	W	60	12.623	66.714	5.890	1.00	23.87	W	O
HETATM	4749	O	HOH	W	61	11.893	47.134	39.605	1.00	23.05	W	O
HETATM	4750	O	HOH	W	62	7.474	40.610	3.914	1.00	31.03	W	O
HETATM	4751	O	HOH	W	63	22.606	52.920	−12.732	1.00	42.64	W	O
HETATM	4752	O	HOH	W	64	2.426	54.692	4.984	1.00	26.28	W	O
HETATM	4753	O	HOH	W	65	48.775	30.973	5.752	1.00	25.77	W	O
HETATM	4754	O	HOH	W	66	−11.173	53.513	23.526	1.00	41.70	W	O
HETATM	4755	O	HOH	W	67	23.529	26.529	24.314	1.00	38.02	W	O

TABLE 2-continued

HETATM	4756	O	HOH	W	68	9.992	28.475	25.594	1.00	34.12	W	O
HETATM	4757	O	HOH	W	69	3.366	44.401	−5.013	1.00	50.58	W	O
HETATM	4758	O	HOH	W	70	34.274	34.206	2.671	1.00	24.77	W	O
HETATM	4759	O	HOH	W	71	20.152	56.215	−4.144	1.00	22.22	W	O
HETATM	4760	O	HOH	W	72	−8.710	24.835	37.208	1.00	27.50	W	O
HETATM	4761	O	HOH	W	73	32.146	41.427	14.964	1.00	28.71	W	O
HETATM	4762	O	HOH	W	74	−19.018	31.978	53.014	1.00	38.25	W	O
HETATM	4763	O	HOH	W	75	0.080	8.693	33.017	1.00	42.67	W	O
HETATM	4764	O	HOH	W	76	−7.947	47.660	19.560	1.00	23.76	W	O
HETATM	4765	O	HOH	W	77	36.529	54.767	10.120	1.00	28.79	W	O
HETATM	4766	O	HOH	W	78	−12.852	35.028	17.783	1.00	25.41	W	O
HETATM	4767	O	HOH	W	79	−0.559	47.749	21.052	1.00	24.10	W	O
HETATM	4768	O	HOH	W	80	−17.156	21.792	34.959	1.00	42.68	W	O
HETATM	4769	O	HOH	W	81	−13.699	23.195	35.641	1.00	33.42	W	O
HETATM	4770	O	HOH	W	82	−9.587	42.543	56.480	1.00	34.56	W	O
HETATM	4771	O	HOH	W	83	43.873	33.067	−8.277	1.00	39.60	W	O
HETATM	4772	O	HOH	W	84	5.761	57.407	37.269	1.00	45.64	W	O
HETATM	4773	O	HOH	W	85	16.884	21.454	20.877	1.00	52.96	W	O
HETATM	4774	O	HOH	W	86	47.763	34.049	1.316	1.00	36.54	W	O
HETATM	4775	O	HOH	W	87	−6.209	31.119	46.066	1.00	44.92	W	O
HETATM	4776	O	HOH	W	88	40.750	51.712	5.730	1.00	33.72	W	O
HETATM	4777	O	HOH	W	89	−21.569	39.844	47.646	1.00	29.53	W	O
HETATM	4778	O	HOH	W	90	26.302	31.299	25.877	1.00	24.97	W	O
HETATM	4779	O	HOH	W	91	−7.619	56.473	35.928	1.00	33.44	W	O
HETATM	4780	O	HOH	W	92	19.370	29.016	−3.829	1.00	36.95	W	O
HETATM	4781	O	HOH	W	93	22.912	21.947	20.348	1.00	34.74	W	O
HETATM	4782	O	HOH	W	94	6.640	33.210	4.482	1.00	25.32	W	O
HETATM	4783	O	HOH	W	95	19.761	65.159	5.818	1.00	28.63	W	O
HETATM	4784	O	HOH	W	96	−2.429	28.740	22.618	1.00	17.06	W	O
HETATM	4785	O	HOH	W	97	−3.064	31.778	42.427	1.00	42.96	W	O
HETATM	4786	O	HOH	W	98	−5.388	7.268	11.141	1.00	30.44	W	O
HETATM	4787	O	HOH	W	99	−22.456	19.371	11.638	1.00	31.53	W	O
HETATM	4788	O	HOH	W	100	4.576	39.683	11.824	1.00	34.42	W	O
HETATM	4789	O	HOH	W	101	−11.699	42.668	37.871	1.00	20.12	W	O
HETATM	4790	O	HOH	W	102	−20.248	30.467	21.517	1.00	43.20	W	O
HETATM	4791	O	HOH	W	103	−2.130	27.300	28.199	1.00	34.69	W	O
HETATM	4792	O	HOH	W	104	−28.854	35.295	32.405	1.00	26.50	W	O
HETATM	4793	O	HOH	W	105	47.956	33.744	15.640	1.00	34.20	W	O
HETATM	4794	O	HOH	W	106	9.854	66.277	−3.306	1.00	36.84	W	O
HETATM	4795	O	HOH	W	107	24.030	38.651	−11.161	1.00	50.50	W	O
HETATM	4796	O	HOH	W	108	48.420	31.498	3.256	1.00	39.12	W	O
HETATM	4797	O	HOH	W	109	−1.253	45.553	15.262	1.00	38.50	W	O
HETATM	4798	O	HOH	W	110	33.843	42.792	13.225	1.00	30.63	W	O
HETATM	4799	O	HOH	W	111	28.703	42.535	−2.829	1.00	30.19	W	O
HETATM	4800	O	HOH	W	112	8.622	12.687	11.102	1.00	29.60	W	O
HETATM	4801	O	HOH	W	113	20.128	67.529	1.352	1.00	33.55	W	O
HETATM	4802	O	HOH	W	114	−0.770	14.323	8.166	1.00	52.45	W	O
HETATM	4803	O	HOH	W	115	−3.656	9.896	7.101	1.00	32.62	W	O
HETATM	4804	O	HOH	W	116	−13.602	22.480	44.154	1.00	35.16	W	O
HETATM	4805	O	HOH	W	117	22.128	20.904	−3.627	1.00	30.87	W	O
HETATM	4806	O	HOH	W	118	−5.070	15.045	27.353	1.00	23.93	W	O
HETATM	4807	O	HOH	W	119	36.061	37.125	23.788	1.00	24.47	W	O
HETATM	4808	O	HOH	W	120	−25.322	30.252	30.726	1.00	41.44	W	O
HETATM	4809	O	HOH	W	121	35.690	29.845	5.576	1.00	16.76	W	O
HETATM	4810	O	HOH	W	122	−24.680	19.112	17.711	1.00	37.84	W	O
HETATM	4811	O	HOH	W	123	13.080	52.502	31.871	1.00	41.89	W	O
HETATM	4812	O	HOH	W	124	2.957	25.901	31.930	1.00	19.65	W	O
HETATM	4813	O	HOH	W	125	39.312	38.534	−13.393	1.00	31.38	W	O
HETATM	4814	O	HOH	W	126	38.067	33.591	−15.755	1.00	35.74	W	O
HETATM	4815	O	HOH	W	127	29.602	55.694	2.224	1.00	36.44	W	O
HETATM	4816	O	HOH	W	128	34.510	31.619	3.906	1.00	29.94	W	O
HETATM	4817	O	HOH	W	129	9.989	23.860	20.084	1.00	32.28	W	O
HETATM	4818	O	HOH	W	130	−17.671	35.139	20.740	1.00	51.29	W	O
HETATM	4819	O	HOH	W	131	36.267	31.168	−11.638	1.00	51.65	W	O
HETATM	4820	O	HOH	W	132	−14.553	50.627	22.253	1.00	36.45	W	O
HETATM	4821	O	HOH	W	133	−16.661	11.632	17.334	1.00	19.62	W	O
HETATM	4822	O	HOH	W	134	23.273	35.371	−10.468	1.00	27.93	W	O
HETATM	4823	O	HOH	W	135	−23.607	44.003	35.480	1.00	29.99	W	O
HETATM	4824	O	HOH	W	136	−11.964	57.410	34.233	1.00	59.88	W	O
HETATM	4825	O	HOH	W	137	−19.087	51.552	39.458	1.00	34.48	W	O
HETATM	4826	O	HOH	W	138	6.012	22.773	15.789	1.00	32.08	W	O
HETATM	4827	O	HOH	W	139	19.642	44.693	−8.548	1.00	30.54	W	O
HETATM	4828	O	HOH	W	140	3.705	36.386	50.313	1.00	38.47	W	O
HETATM	4829	O	HOH	W	141	1.298	37.283	7.120	1.00	51.13	W	O
HETATM	4830	O	HOH	W	142	−23.191	29.343	32.125	1.00	50.13	W	O
HETATM	4831	O	HOH	W	143	46.067	49.093	7.670	1.00	42.60	W	O
HETATM	4832	O	HOH	W	144	31.146	48.281	12.422	1.00	40.48	W	O
HETATM	4833	O	HOH	W	145	31.480	33.377	27.417	1.00	40.50	W	O
HETATM	4834	O	HOH	W	146	−0.521	7.311	18.965	1.00	40.93	W	O
HETATM	4835	O	HOH	W	147	4.938	47.003	20.293	1.00	35.68	W	O

TABLE 2-continued

HETATM	4836	O	HOH	W	148	2.572	56.018	12.990	1.00	38.20	W	O
HETATM	4837	O	HOH	W	149	4.166	41.330	46.439	1.00	51.22	W	O
HETATM	4838	O	HOH	W	150	−27.096	42.038	36.548	1.00	54.71	W	O
HETATM	4839	O	HOH	W	151	−9.606	44.717	20.161	1.00	26.34	W	O
HETATM	4840	O	HOH	W	152	−12.543	24.530	50.664	1.00	31.97	W	O
HETATM	4841	O	HOH	W	153	23.986	57.755	13.449	1.00	41.58	W	O
HETATM	4842	O	HOH	W	154	4.142	48.610	−7.954	1.00	41.73	W	O
HETATM	4843	O	HOH	W	155	−8.571	34.493	10.496	1.00	35.68	W	O
HETATM	4844	O	HOH	W	156	6.535	43.683	−0.301	1.00	28.35	W	O
HETATM	4845	O	HOH	W	157	5.098	9.837	31.389	1.00	32.69	W	O
HETATM	4846	O	HOH	W	158	4.605	38.451	46.567	1.00	44.80	W	O
HETATM	4847	O	HOH	W	159	−12.373	9.262	29.626	1.00	43.00	W	O
HETATM	4848	O	HOH	W	160	21.944	64.392	14.788	1.00	43.27	W	O
HETATM	4849	O	HOH	W	161	8.410	42.221	0.553	1.00	38.42	W	O
HETATM	4850	O	HOH	W	162	−15.092	24.451	51.951	1.00	33.87	W	O
HETATM	4851	O	HOH	W	163	−28.497	40.660	38.549	1.00	42.45	W	O
HETATM	4852	O	HOH	W	164	4.677	56.197	15.176	1.00	39.88	W	O
HETATM	4853	O	HOH	W	165	9.008	31.037	17.696	1.00	37.12	W	O
HETATM	4854	O	HOH	W	166	−13.943	48.188	19.442	1.00	51.59	W	O
HETATM	4855	O	HOH	W	167	−16.372	52.024	18.619	1.00	30.94	W	O
HETATM	4856	O	HOH	W	168	36.587	31.130	−14.714	1.00	37.59	W	O
HETATM	4857	O	HOH	W	169	40.198	33.790	−13.561	1.00	51.85	W	O
HETATM	4858	O	HOH	W	170	11.326	50.791	32.880	1.00	41.20	W	O
HETATM	4859	O	HOH	W	171	24.824	41.289	−12.891	1.00	48.97	W	O
HETATM	4860	O	HOH	W	172	−19.243	31.094	23.985	1.00	65.07	W	O
HETATM	4861	O	HOH	W	173	22.235	20.511	18.399	1.00	35.72	W	O
HETATM	4862	O	HOH	W	174	25.487	19.422	20.119	1.00	42.44	W	O
HETATM	4863	O	HOH	W	175	−0.531	31.883	14.385	1.00	36.04	W	O
HETATM	4864	O	HOH	W	176	21.134	46.888	6.137	1.00	20.06	W	O
END												

SEQUENCE LISTING

<160> NUMBER OF SEQ ID NOS: 8

<210> SEQ ID NO 1
<211> LENGTH: 1124
<212> TYPE: PRT
<213> ORGANISM: Homo sapiens

<400> SEQUENCE: 1

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Met Ala Pro Pro Ser Glu Glu Thr Pro Leu Ile Pro Gln Arg Ser Cys
  1               5                  10                  15

Ser Leu Leu Ser Thr Glu Ala Gly Ala Leu His Val Leu Leu Pro Ala
             20                  25                  30

Arg Gly Pro Gly Pro Pro Gln Arg Leu Ser Phe Ser Phe Gly Asp His
         35                  40                  45

Leu Ala Glu Asp Leu Cys Val Gln Ala Ala Lys Ala Ser Gly Ile Leu
     50                  55                  60

Pro Val Tyr His Ser Leu Phe Ala Leu Ala Thr Glu Asp Leu Ser Cys
 65                  70                  75                  80

Trp Phe Pro Pro Ser His Ile Phe Ser Val Glu Asp Ala Ser Thr Gln
                 85                  90                  95

Val Leu Leu Tyr Arg Ile Arg Phe Tyr Phe Pro Asn Trp Phe Gly Leu
            100                 105                 110

Glu Lys Cys His Arg Phe Gly Leu Arg Lys Asp Leu Ala Ser Ala Ile
        115                 120                 125

Leu Asp Leu Pro Val Leu Glu His Leu Phe Ala Gln His Arg Ser Asp
    130                 135                 140

Leu Val Ser Gly Arg Leu Pro Val Gly Leu Ser Leu Lys Glu Gln Gly
145                 150                 155                 160

Glu Cys Leu Ser Leu Ala Val Leu Asp Leu Ala Arg Met Ala Arg Glu
                165                 170                 175
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Gln Ala Gln Arg Pro Gly Glu Leu Leu Lys Thr Val Ser Tyr Lys Ala
            180                 185                 190

Cys Leu Pro Pro Ser Leu Arg Asp Leu Ile Gln Gly Leu Ser Phe Val
        195                 200                 205

Thr Arg Arg Arg Ile Arg Arg Thr Val Arg Arg Ala Leu Arg Arg Val
    210                 215                 220

Ala Ala Cys Gln Ala Asp Arg His Ser Leu Met Ala Lys Tyr Ile Met
225                 230                 235                 240

Asp Leu Glu Arg Leu Asp Pro Ala Gly Ala Ala Glu Thr Phe His Val
                245                 250                 255

Gly Leu Pro Gly Ala Leu Gly Gly His Asp Gly Leu Gly Leu Leu Arg
            260                 265                 270

Val Ala Gly Asp Gly Gly Ile Ala Trp Thr Gln Gly Glu Gln Glu Val
        275                 280                 285

Leu Gln Pro Phe Cys Asp Phe Pro Glu Ile Val Asp Ile Ser Ile Lys
    290                 295                 300

Gln Ala Pro Arg Val Gly Pro Ala Gly Glu His Arg Leu Val Thr Val
305                 310                 315                 320

Thr Arg Thr Asp Asn Gln Ile Leu Glu Ala Glu Phe Pro Gly Leu Pro
                325                 330                 335

Glu Ala Leu Ser Phe Val Ala Leu Val Asp Gly Tyr Phe Arg Leu Thr
            340                 345                 350

Thr Asp Ser Gln His Phe Phe Cys Lys Glu Val Ala Pro Pro Arg Leu
        355                 360                 365

Leu Glu Glu Val Ala Glu Gln Cys His Gly Pro Ile Thr Leu Asp Phe
    370                 375                 380

Ala Ile Asn Lys Leu Lys Thr Gly Gly Ser Arg Pro Gly Ser Tyr Val
385                 390                 395                 400

Leu Arg Arg Ser Pro Gln Asp Phe Asp Ser Phe Leu Leu Thr Val Cys
                405                 410                 415

Val Gln Asn Pro Leu Gly Pro Asp Tyr Lys Gly Cys Leu Ile Arg Arg
            420                 425                 430

Ser Pro Thr Gly Thr Phe Leu Leu Val Gly Leu Ser Arg Pro His Ser
        435                 440                 445

Ser Leu Arg Glu Leu Leu Ala Thr Cys Trp Asp Gly Gly Leu His Val
    450                 455                 460

Asp Gly Val Ala Val Thr Leu Thr Ser Cys Cys Ile Pro Arg Pro Lys
465                 470                 475                 480

Glu Lys Ser Asn Leu Ile Val Val Gln Arg Gly His Ser Pro Pro Thr
                485                 490                 495

Ser Ser Leu Val Gln Pro Gln Ser Gln Tyr Gln Leu Ser Gln Met Thr
            500                 505                 510

Phe His Lys Ile Pro Ala Asp Ser Leu Glu Trp His Glu Asn Leu Gly
        515                 520                 525

His Gly Ser Phe Thr Lys Ile Tyr Arg Gly Cys Arg His Glu Val Val
    530                 535                 540

Asp Gly Glu Ala Arg Lys Thr Glu Val Leu Leu Lys Val Met Asp Ala
545                 550                 555                 560

Lys His Lys Asn Cys Met Glu Ser Phe Leu Glu Ala Ala Ser Leu Met
                565                 570                 575

Ser Gln Val Ser Tyr Arg His Leu Val Leu Leu His Gly Val Cys Met
            580                 585                 590

Ala Gly Asp Ser Thr Met Val Gln Glu Phe Val His Leu Gly Ala Ile
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595 600 605

Asp Met Tyr Leu Arg Lys Arg Gly His Leu Val Pro Ala Ser Trp Lys
610 615 620

Leu Gln Val Val Lys Gln Leu Ala Tyr Ala Leu Asn Tyr Leu Glu Asp
625 630 635 640

Lys Gly Leu Pro His Gly Asn Val Ser Ala Arg Lys Val Leu Leu Ala
645 650 655

Arg Glu Gly Ala Asp Gly Ser Pro Pro Phe Ile Lys Leu Ser Asp Pro
660 665 670

Gly Val Ser Pro Ala Val Leu Ser Leu Glu Met Leu Thr Asp Arg Ile
675 680 685

Pro Trp Val Ala Pro Glu Cys Leu Arg Glu Ala Gln Thr Leu Ser Leu
690 695 700

Glu Ala Asp Lys Trp Gly Phe Gly Ala Thr Val Trp Glu Val Phe Ser
705 710 715 720

Gly Val Thr Met Pro Ile Ser Ala Leu Asp Pro Ala Lys Lys Leu Gln
725 730 735

Phe Tyr Glu Asp Arg Gln Gln Leu Pro Ala Pro Lys Trp Thr Glu Leu
740 745 750

Ala Leu Leu Ile Gln Gln Cys Met Ala Tyr Glu Pro Val Gln Arg Pro
755 760 765

Ser Phe Arg Ala Val Ile Arg Asp Leu Asn Ser Leu Ile Ser Ser Asp
770 775 780

Tyr Glu Leu Leu Ser Asp Pro Thr Pro Gly Ala Leu Ala Pro Arg Asp
785 790 795 800

Gly Leu Trp Asn Gly Ala Gln Leu Tyr Ala Cys Gln Asp Pro Thr Ile
805 810 815

Phe Glu Glu Arg His Leu Lys Tyr Ile Ser Gln Leu Gly Lys Gly Asn
820 825 830

Phe Gly Ser Val Glu Leu Cys Arg Tyr Asp Pro Leu Gly Asp Asn Thr
835 840 845

Gly Ala Leu Val Ala Val Lys Gln Leu Gln His Ser Gly Pro Asp Gln
850 855 860

Gln Arg Asp Phe Gln Arg Glu Ile Gln Ile Leu Lys Ala Leu His Ser
865 870 875 880

Asp Phe Ile Val Lys Tyr Arg Gly Val Ser Tyr Gly Pro Gly Arg Gln
885 890 895

Ser Leu Arg Leu Val Met Glu Tyr Leu Pro Ser Gly Cys Leu Arg Asp
900 905 910

Phe Leu Gln Arg His Arg Ala Arg Leu Asp Ala Ser Arg Leu Leu Leu
915 920 925

Tyr Ser Ser Gln Ile Cys Lys Gly Met Glu Tyr Leu Gly Ser Arg Arg
930 935 940

Cys Val His Arg Asp Leu Ala Ala Arg Asn Ile Leu Val Glu Ser Glu
945 950 955 960

Ala His Val Lys Ile Ala Asp Phe Gly Leu Ala Lys Leu Leu Pro Leu
965 970 975

Asp Lys Asp Tyr Tyr Val Val Arg Glu Pro Gly Gln Ser Pro Ile Phe
980 985 990

Trp Tyr Ala Pro Glu Ser Leu Ser Asp Asn Ile Phe Ser Arg Gln Ser
995 1000 1005

Asp Val Trp Ser Phe Gly Val Val Leu Tyr Glu Leu Phe Thr Tyr Cys
1010 1015 1020

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Asp Lys Ser Cys Ser Pro Ser Ala Glu Phe Leu Arg Met Met Gly Cys
1025               1030                1035                1040

Glu Arg Asp Val Pro Ala Leu Cys Arg Leu Leu Glu Leu Leu Glu Glu
               1045                1050                1055

Gly Gln Arg Leu Pro Ala Pro Pro Ala Cys Pro Ala Glu Val His Glu
           1060                1065                1070

Leu Met Lys Leu Cys Trp Ala Pro Ser Pro Gln Asp Arg Pro Ser Phe
       1075                1080                1085

Ser Ala Leu Gly Pro Gln Leu Asp Met Leu Trp Ser Gly Ser Arg Gly
   1090                1095                1100

Cys Glu Thr His Ala Phe Thr Ala His Pro Glu Gly Lys His His Ser
1105               1110                1115                1120

Leu Ser Phe Ser
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<210> SEQ ID NO 2
<211> LENGTH: 72
<212> TYPE: PRT
<213> ORGANISM: Homo sapiens

<400> SEQUENCE: 2

Asp Phe Gly Leu Met Arg Ala Leu Pro Gln Asn Asp Asp His Tyr Val
  1               5                  10                  15

Met Gln Glu His Arg Lys Val Pro Phe Ala Trp Cys Ala Pro Glu Ser
             20                  25                  30

Leu Lys Thr Arg Thr Phe Ser His Ala Ser Asp Thr Trp Met Phe Gly
         35                  40                  45

Val Thr Leu Trp Glu Met Phe Thr Tyr Gly Gln Glu Pro Trp Ile Gly
     50                  55                  60

Leu Asn Gly Ser Gln Ile Leu His
 65                  70


<210> SEQ ID NO 3
<211> LENGTH: 67
<212> TYPE: PRT
<213> ORGANISM: Homo sapiens

<400> SEQUENCE: 3

Asp Phe Gly Leu Ser Arg Asn Ile Tyr Ser Ala Asp Tyr Tyr Lys Asp
  1               5                  10                  15

Ala Ile Pro Ile Arg Trp Met Pro Pro Glu Ser Ile Phe Tyr Asn Arg
             20                  25                  30

Tyr Thr Thr Glu Ser Asp Val Trp Ala Tyr Gly Val Val Leu Trp Glu
         35                  40                  45

Ile Phe Ser Tyr Gly Leu Gln Pro Tyr Tyr Gly Met Ala His Glu Glu
     50                  55                  60

Val Ile Tyr
 65


<210> SEQ ID NO 4
<211> LENGTH: 71
<212> TYPE: PRT
<213> ORGANISM: Homo sapiens

<400> SEQUENCE: 4

Asp Phe Gly Met Thr Arg Asp Ile Tyr Glu Thr Asp Tyr Tyr Arg Lys
  1               5                  10                  15

Gly Gly Lys Gly Leu Leu Pro Val Arg Trp Met Ala Pro Glu Ser Leu
             20                  25                  30
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Lys Asp Gly Val Phe Thr Thr Ser Ser Asp Met Trp Ser Phe Gly Val
35 40 45

Val Leu Trp Glu Ile Thr Ser Leu Ala Glu Gln Pro Tyr Gln Gly Leu
50 55 60

Ser Asn Glu Gln Val Leu Lys
65 70

<210> SEQ ID NO 5
<211> LENGTH: 71
<212> TYPE: PRT
<213> ORGANISM: Homo sapiens

<400> SEQUENCE: 5

Asp Phe Gly Leu Ala Arg Asp Ile His His Ile Asp Tyr Tyr Lys Lys
1 5 10 15

Thr Thr Asn Gly Arg Leu Pro Val Lys Trp Met Ala Pro Glu Ala Leu
20 25 30

Phe Asp Arg Ile Tyr Thr His Gln Ser Asp Val Trp Ser Phe Gly Val
35 40 45

Leu Leu Trp Glu Ile Phe Thr Leu Gly Gly Ser Pro Tyr Pro Gly Val
50 55 60

Pro Val Glu Glu Leu Phe Lys
65 70

<210> SEQ ID NO 6
<211> LENGTH: 70
<212> TYPE: PRT
<213> ORGANISM: Homo sapiens

<400> SEQUENCE: 6

Asp Phe Gly Leu Ala Arg Leu Ile Glu Asp Asn Glu Tyr Thr Ala Arg
1 5 10 15

Gln Gly Ala Lys Phe Pro Ile Lys Trp Thr Ala Pro Glu Ala Ala Leu
20 25 30

Tyr Gly Arg Phe Thr Ile Lys Ser Asp Val Trp Ser Phe Gly Ile Leu
35 40 45

Leu Thr Glu Leu Thr Thr Lys Gly Arg Val Pro Tyr Pro Gly Met Val
50 55 60

Asn Arg Glu Val Leu Asp
65 70

<210> SEQ ID NO 7
<211> LENGTH: 6
<212> TYPE: PRT
<213> ORGANISM: Artificial Sequence
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<210> SEQ ID NO 8
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Glu Glu Glu Glu Tyr
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We claim:

1. A method for identifying a candidate inhibitor using three-dimensional structure coordinates generated from a human Janus Kinase 3 crystal comprising a human Janus Kinase 3 protein,

wherein said human Janus Kinase 3 protein consists of amino acid residues 810-1115 of SEQ ID NO: 1,

wherein said human Janus Kinase 3 protein comprises a kinase domain,

wherein said human Janus Kinase 3 kinase domain is in complex with a chemical entity selected from the group consisting of adenosine, ATP, an ATP analogue, AMP-PNP, a nucleotide triphosphate, a nucleotide diphosphate, and phosphate, and

wherein said method comprises:

(a) generating a three-dimensional structure on a computer of a molecular complex comprising a binding site of amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn832, Phe833, Gly834, Ser835, Val836 Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907 Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Glu985, Gln988, Ser989, Pro990 and Trp993 according to Table 2, wherein the root mean square deviation of the backbone atoms is not greater than about 2.5 Å;

(b) employing said three-dimensional structure to design or select said candidate inhibitor; and

(c) contacting said candidate inhibitor with human Janus Kinase 3 to determine the ability of said candidate inhibitor to bind to human Janus Kinase 3.

2. The method according to claim **1**, wherein said chemical entity is AMP-PNP.

3. A method for identifying a candidate inhibitor using a human Janus Kinase 3 crystal comprising a human Janus Kinase 3 protein,

wherein said human Janus Kinase 3 protein consists of amino acid residues 810-1115 of SEQ ID NO: 1,

wherein said human Janus Kinase 3 protein comprises a kinase domain,

wherein said human Janus Kinase 3 kinase domain is in complex with a chemical entity selected from the group consisting of adenosine, ATP, an ATP analogue, AMP-PNP, a nucleotide triphosphate, a nucleotide diphosphate, and phosphate, and wherein said crystal is characterized by either: (i) space group $P2_1$ and has unit cell parameters of a=59.98±4 Å, b=90.19±4 Å, c=69.00±4 Å, α=90°, β=111.5°, γ=90°, or (ii) space group $P2_12_12_1$ and has unit cell parameters of a=72.36±4 Å, b=90.04±4 Å, c=105.60±4 Å, α=β=γ=90°,

wherein said method comprises:

(a) soaking said human Janus Kinase 3 crystal in the presence of said candidate inhibitor thereby displacing said chemical entity and generating a human Janus Kinase 3 crystal comprising a human Janus Kinase 3 kinase domain in complex with said candidate inhibitor;

(b) determining the three-dimensional structure coordinates of human Janus Kinase 3 using the crystal in step (a);

(c) using the structure coordinates from step (b) to generate a three-dimensional structure of a molecular complex comprising a binding site of amino acid residues Gln827, Leu828, Gly829, Lys830, Gly831, Asn832, Phe833, Gly834, Ser835, Val836, Glu837, Leu838, Val852, Ala853, Val854, Lys855, Gln856, Leu857, Val884, Lys885, Tyr886, Leu900, Val901, Met902, Glu903, Tyr904, Leu905, Pro906, Ser907, Gly908, Cys909, Leu910, Arg911, Asp912, His947, Asp949, Leu950, Ala951, Ala952, Arg953, Asn954, Ile955, Leu956, Val957, Ala966, Asp967, Leu970, Glu985, Gln988, Ser989, Pro990 and Trp993 according to Table 2, wherein the root mean square deviation of the backbone atoms is not greater than about 2.5 Å; and

(d) contacting said candidate inhibitor with human Janus Kinase 3 to determine the ability of said candidate inhibitor to bind to human Janus Kinase 3.

4. The method according to claim **3**, wherein said chemical entity is AMP-PNP.

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